Stanford CS224W: Reasoning over Knowledge Graphs

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

ANNOUNCEMENTS

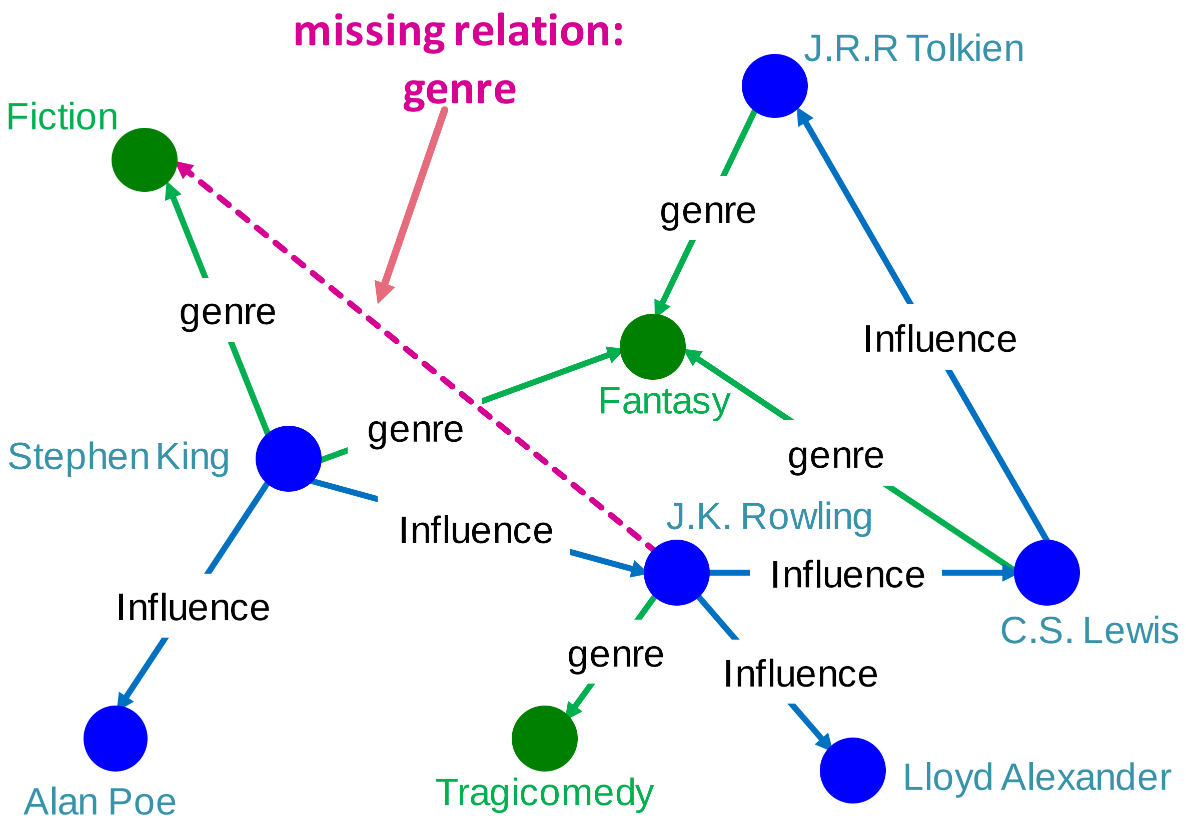
- We received comments regarding office hour logistics, and decided to make the following adjustments
- We will add an **evening OH on Monday 7pm**
- We will impose a **10-minute time limit for each student**
- We will create **breakout rooms for students to discuss specific questions**

Recap: KG Completion Task

Given an enormous KG, can we complete the KG?

- For a given (**head**, **relation**), we predict missing **tails**.
  - (Note this is slightly different from link prediction task)

Example task: Predict the tail "Science Fiction" for ("J.K. Rowling", "genre")

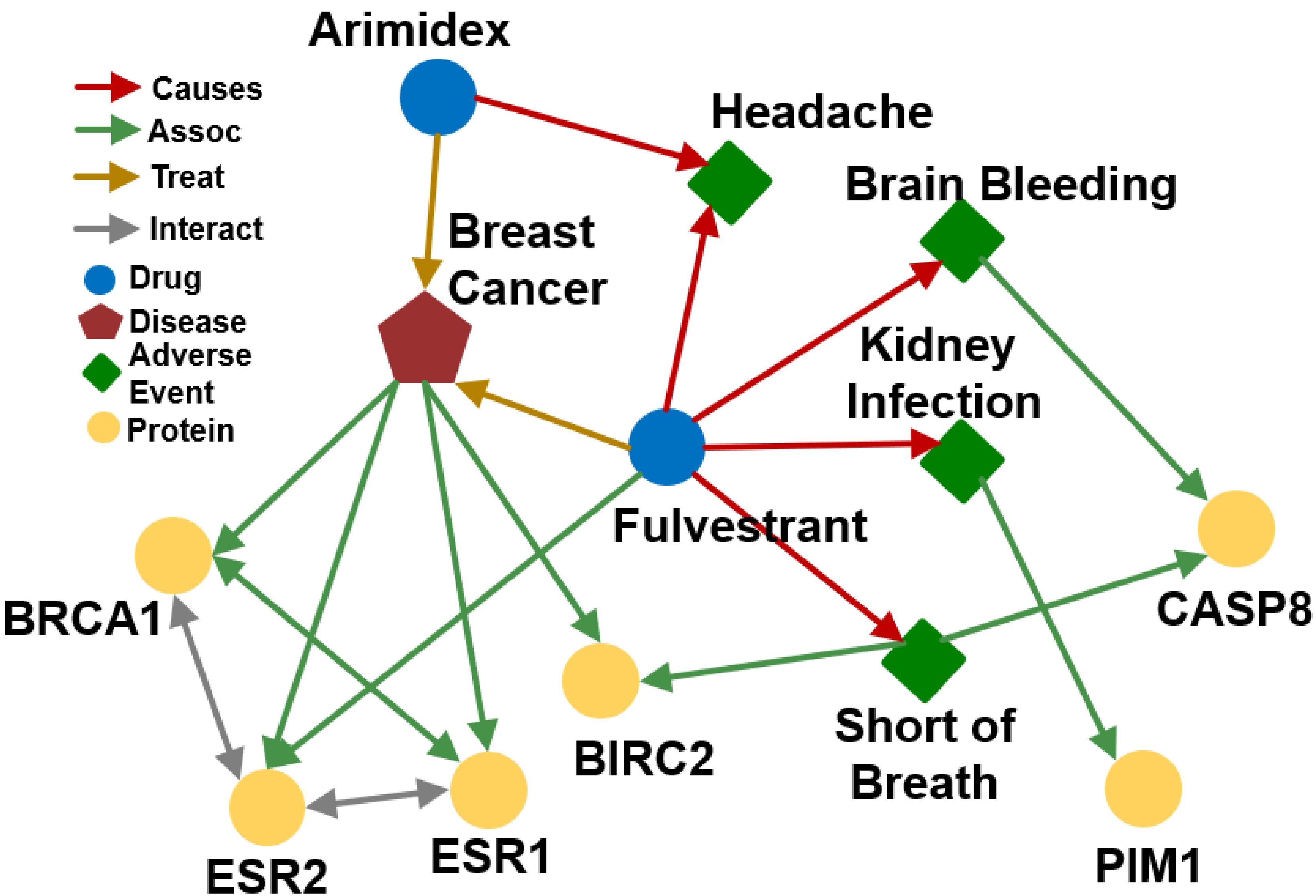


Today: Reasoning over KGs

- **Goal**:
  - How to perform multi-hop reasoning over KGs?

- **Reasoning over Knowledge Graphs**
  - Answering multi-hop queries
    - Path Queries
    - Conjunctive Queries
  - Query2Box

Example KG: Biomedicine

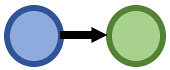


Predictive Queries on KG

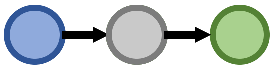
Can we do multi-hop reasoning, i.e., answer complex queries on an incomplete, massive KG?

Query Types	Examples: Natural Language Question, Query
One-hop Queries	What adverse event is caused by Fulvestrant? (e:Fulvestrant, (r:Causes))
Path Queries	What protein is associated with the adverse event caused by Fulvestrant? (e:Fulvestrant, (r:Causes, r:Assoc))
Conjunctive Queries	What is the drug that treats breast cancer and caused headache? ((e:BreastCancer, (r:TreatedBy)), (e:Migraine, (r:CausedBy))

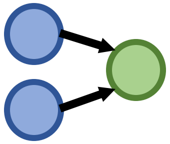
In this lecture, we only focus on answering queries on a KG!
The notation will be detailed next.



One-hop Queries



Path Queries



Conjunctive Queries

Predictive One-hop Queries

- **We can formulate knowledge graph completion problems as answering one-hop queries.**

- **KG completion:** Is link (h, r, t) in the KG?

$$\Updownarrow$$

- **One-hop query:** Is t an answer to query (h, r)?
  - **For example:** What side effects are caused by drug Fulvestrant?

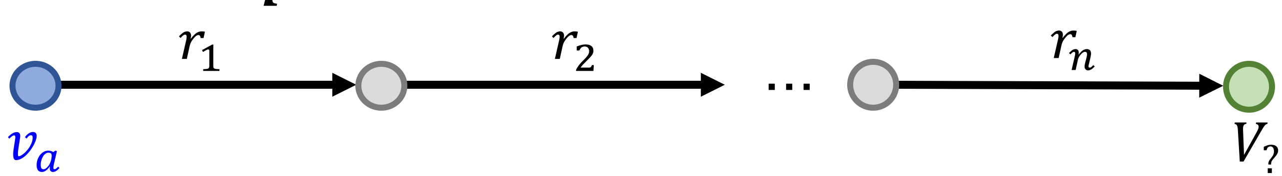
Path Queries

- Generalize one-hop queries to path queries by **adding more relations on the path**.
- An n-hop path query q can be represented by

$$q = (v_a, (r_1, \dots, r_n))$$

  - v_a is an "anchor" entity,
  - Let answers to q in graph G be denoted by $[\![q]\!]_G$.

Query Plan of q:

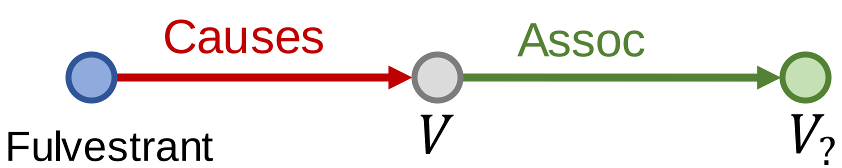


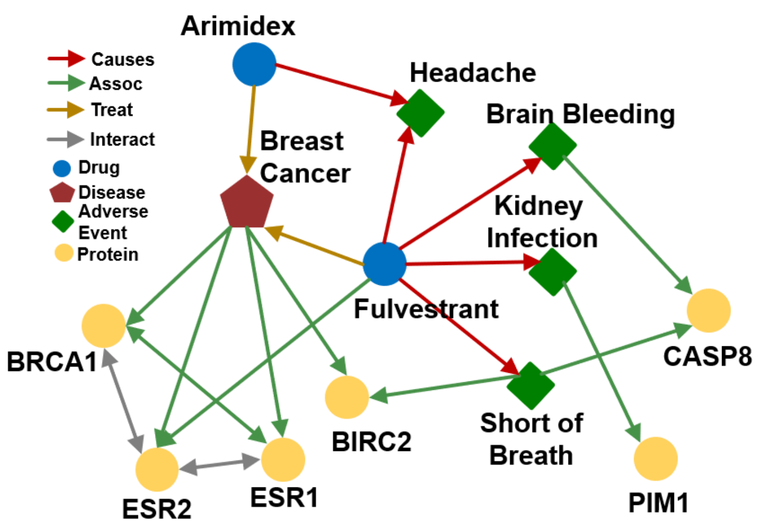
Query plan of path queries is a chain.

Path Queries

Question: “*What proteins are **associated** with adverse events **caused** by **Fulvestrant**?*”

- v_a is **e:Fulvestrant**
- (r_1, r_2) is (**r:Causes**, **r:Assoc**)
- **Query:** (**e:Fulvestrant**, (**r:Causes**, **r:Assoc**))



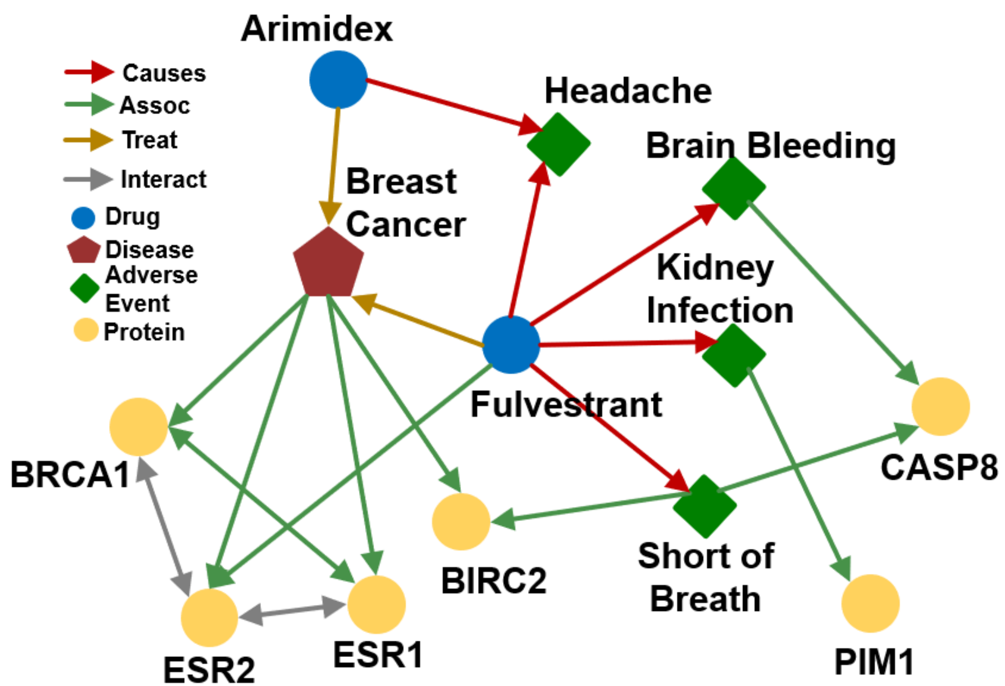


Path Queries

Question: "*What proteins are **associated** with adverse events **caused** by **Fulvestrant**?*"

- **Query: (e:Fulvestrant, (r:Causes, r:Assoc))**

Given a KG, how to answer a path query?



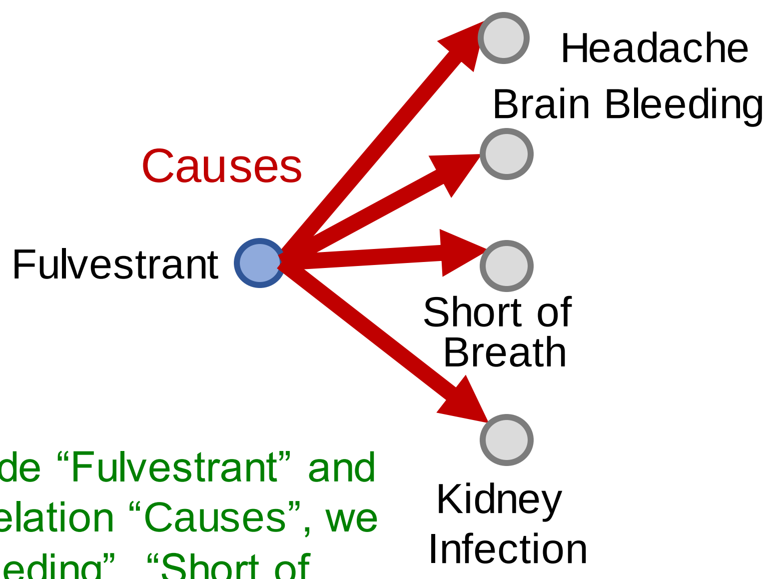
Traversing Knowledge Graphs

- **We answer path queries by traversing the KG:** *"What proteins are **associated** with adverse events **caused** by **Fulvestrant**?"*
- **Query:** (e:Fulvestrant, (r:Causes, r:Assoc))

Start from the **anchor node** (Fulvestrant).

Traversing Knowledge Graphs

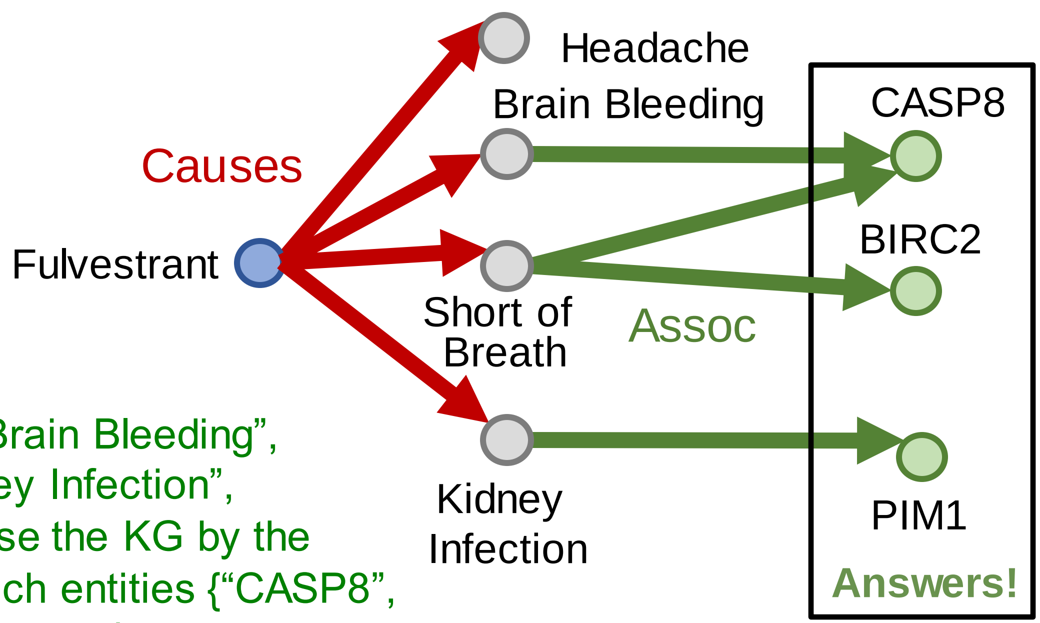
- **We answer path queries by traversing the KG:** *"What proteins are **associated** with adverse events **caused** by **Fulvestrant**?"*
- **Query:** (e:Fulvestrant, (r:Causes, r:Assoc))



Start from the anchor node "Fulvestrant" and traverse the KG by the relation "Causes", we reach entities {"Brain Bleeding", "Short of Breath", "Kidney Infection", "Headache"}.

Traversing Knowledge Graphs

- **We answer path queries by traversing the KG:**
  "What proteins are ***associated*** *with adverse events* ***caused*** *by* ***Fulvestrant****?"*
- **Query: (e:Fulvestrant, (r:Causes, r:Assoc))**



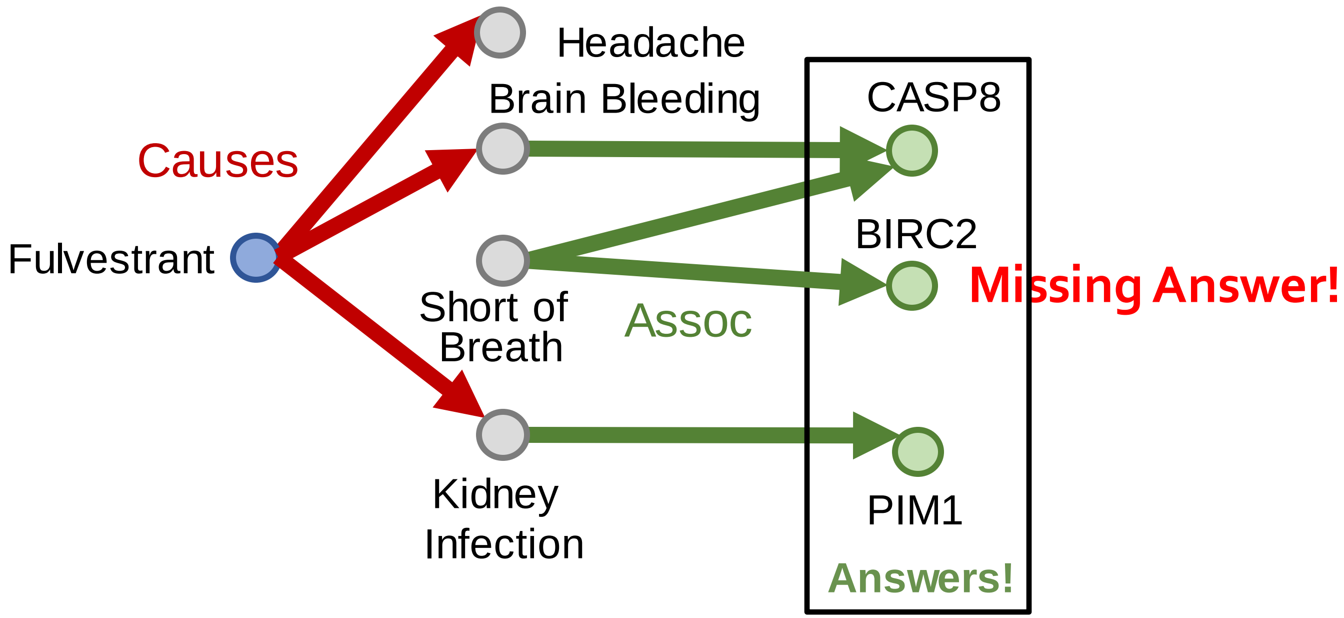
Start from the nodes {"Brain Bleeding", "Short of Breath", "Kidney Infection", "Headache"} and traverse the KG by the relation "Assoc", we reach entities {"CASP8", "BIRC2", "PIM1"}. These are the answers.

However, KGs are incomplete

- **Answering queries seems easy: Just traverse the graph.**
- **But KGs are incomplete and unknown:**
  - Many relations between entities are missing or are incomplete
    - For example, we lack all the biomedical knowledge
    - Enumerating all the facts takes non-trivial time and cost, we cannot hope that KGs will ever be fully complete
- **Due to KG incompleteness, one is not able to identify all the answer entities**

Example: Incomplete KG

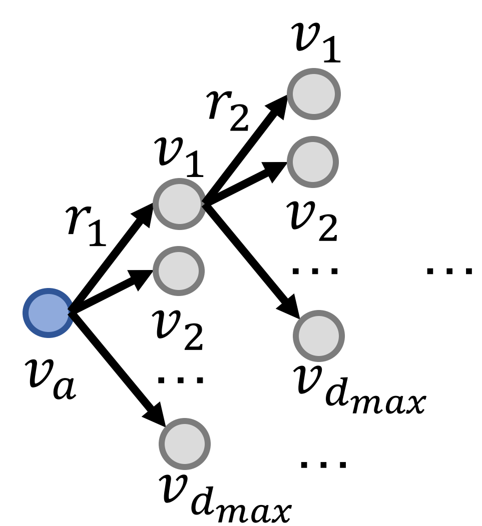
- **We answer path queries by traversing the KG:** *"What proteins are **associated** with adverse events **caused** by **Fulvestrant**?"*
- **Query: (e:Fulvestrant, (r:Causes, r:Assoc))**



Can KG Completion Help?

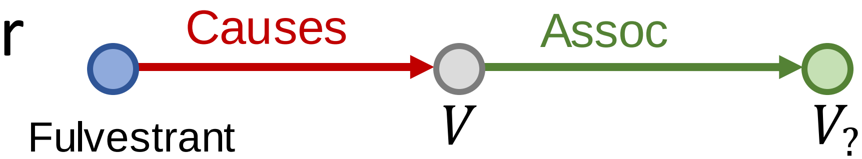
Can we first do KG completion and then traverse the completed (probabilistic) KG?

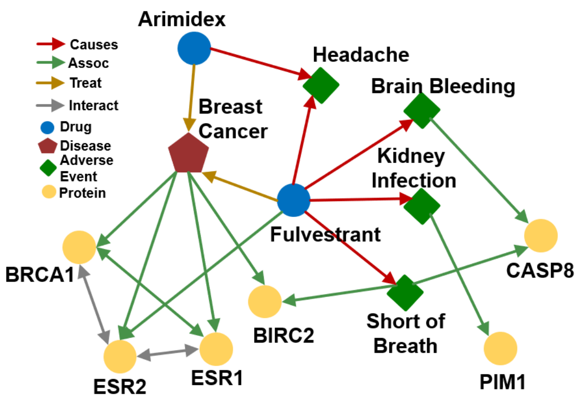
- **No!** The "completed" KG is a **dense graph**!
  - Most (h, r, t) triples (edge on KG) will have some non-zero probability.
- Time complexity of traversing a dense KG is exponential as a function of the path length L: $O(d_{max}^L)$



Task: Predictive Queries

- We need a way to answer path-based queries over an incomplete knowledge graph.
- We want our approach to implicitly impute and account for the incomplete KG.
- **Task: Predictive queries**
  - Want to be able to answer arbitrary queries while implicitly imputing for the missing information
  - **Generalization of the link prediction task**





Outline of the Lecture

1) Given entity embeddings, how do we answer an arbitrary query?

- Path queries: Using a generalization of TransE
- Conjunctive queries: Using Query2Box
- And-Or Queries: Using Query2Box and query rewriting

(We will assume entity embeddings and relation embeddings are given)

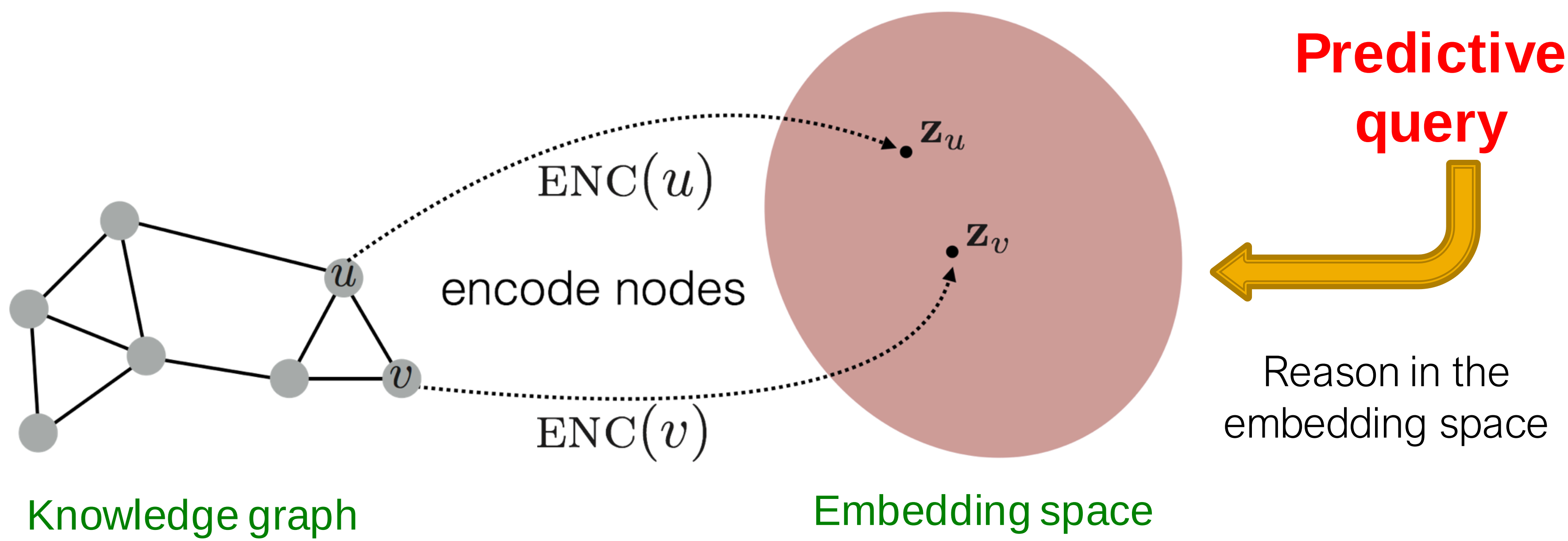
2) How do we train the embeddings?

- The process of determining entity and relation embeddings which allow us to embed a query.

Stanford CS224W: Answering Predictive Queries on Knowledge Graphs

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

General Idea



Map queries into embedding space. **Learn to reason in that space**

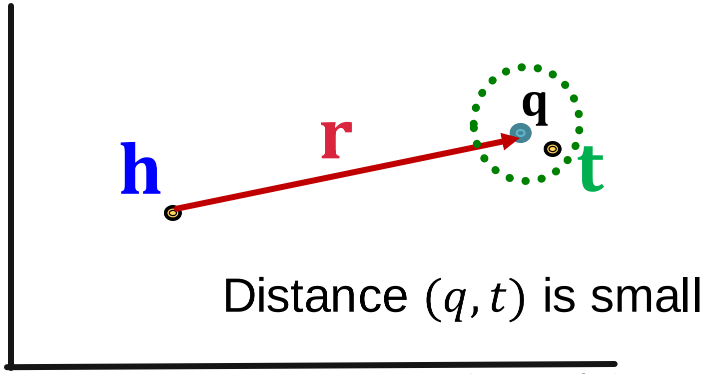
- Embed query into a single **point** in the Euclidean space: answer nodes are close to the query.
- **Query2Box:** Embed query into a hyper-rectangle (**box**) in the Euclidean space: answer nodes are enclosed in the box.

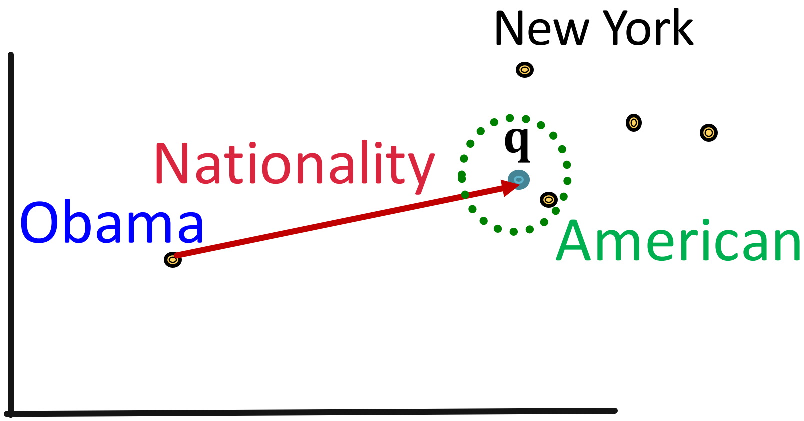
[Embedding Logical Queries on Knowledge Graphs. Hamilton, et al., NeurIPS 2018]
[Query2box: Reasoning over Knowledge Graphs in Vector Space Using Box Embeddings. Ren, et al., ICLR 2020]

Idea: Traversing KG in Vector Space

- **Key idea: Embed queries!**
  - Generalize **TransE** to multi-hop reasoning.
  - **Recap: TransE:** Translate $\mathbf{h}$ to $\mathbf{t}$ using $\mathbf{r}$ with score function $f_r(h,t) = -||\mathbf{h} + \mathbf{r} - \mathbf{t}||$.
  - Another way to interpret this is that:
    - **Query embedding**: $\mathbf{q} = \mathbf{h} + \mathbf{r}$
    - Goal: **query embedding** $\mathbf{q}$ is **close** to the **answer embedding** $\mathbf{t}$

$$f_q(t) = -||\mathbf{q} - \mathbf{t}||$$

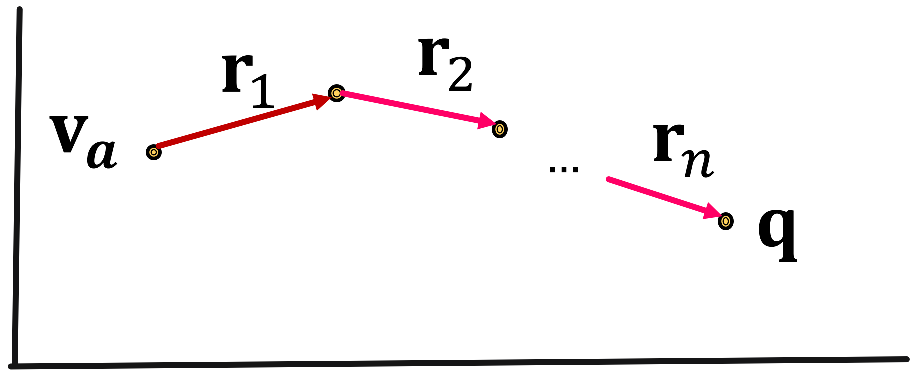




Traversing KG in Vector Space

- **Key idea: Embed queries!**
  - Generalize **TransE** to multi-hop reasoning.

Given a path query $q = (v_a, (r_1, \dots, r_n))$,



$$\mathbf{q} = \mathbf{v}_a + \mathbf{r}_1 + \cdots + \mathbf{r}_n$$

- The embedding process **only involves vector addition**, **independent of # entities** in the KG!

Traversing KG in Vector Space (1)

Embed path queries in vector space.

- **Question:** "*What proteins are **associated** with adverse events **caused** by **Fulvestrant**?*"
- **Query:** (**e:Fulvestrant**, (**r:Causes** , **r:Assoc**))

Follow the query plan:

Query Plan | **Embedding Process**

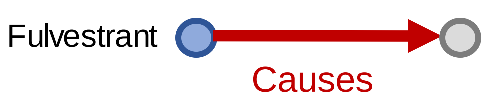
Traversing KG in Vector Space (2)

Embed path queries in vector space.

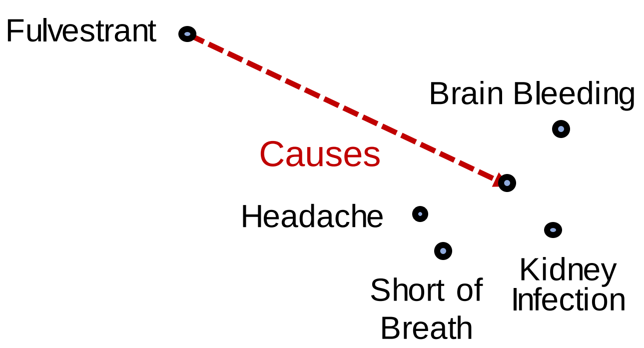
- **Question:** "*What proteins are **associated** with adverse events **caused** by **Fulvestrant**?*"
- **Query:** (**e:Fulvestrant**, (**r:Causes** , **r:Assoc**))

Follow the query plan:

Query Plan



Embedding Process



Traversing KG in Vector Space (3)

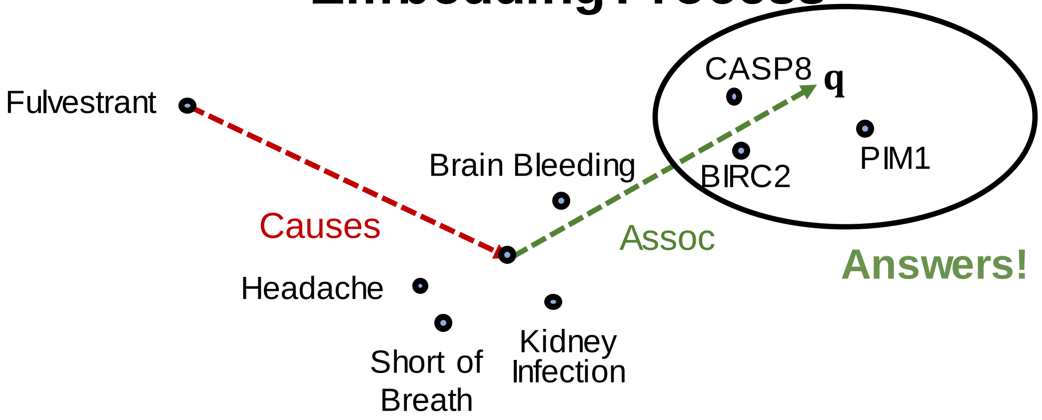
Embed path queries in vector space.

- **Question:** "*What proteins are **associated** with adverse events **caused** by **Fulvestrant**?*"
- **Query:** (**e:Fulvestrant**, (**r:Causes** , **r:Assoc**))

Follow the query plan:

Query Plan

Embedding Process



Traversing KG in Vector Space (4)

Insights:

- We can train **TransE** to optimize knowledge graph completion objective (Lecture 11)
- Since **TransE** can naturally handle **compositional relations**, it can handle path queries by translating in the latent space **for multiple hops using addition of relation embeddings**.
- For **TransR** / **DistMult** / **ComplEx**, since they cannot handle compositional relations, they cannot be easily extended to handle **path queries**.

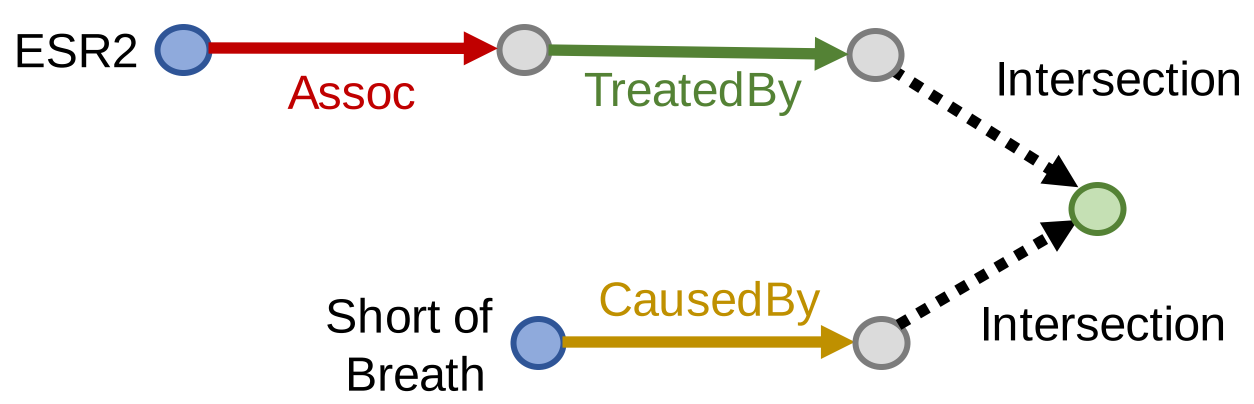
Conjunctive Queries

Can we answer **more complex queries with logic conjunction operation**?

- **Conjunctive Queries:** *"What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?"*

((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))

Query plan:

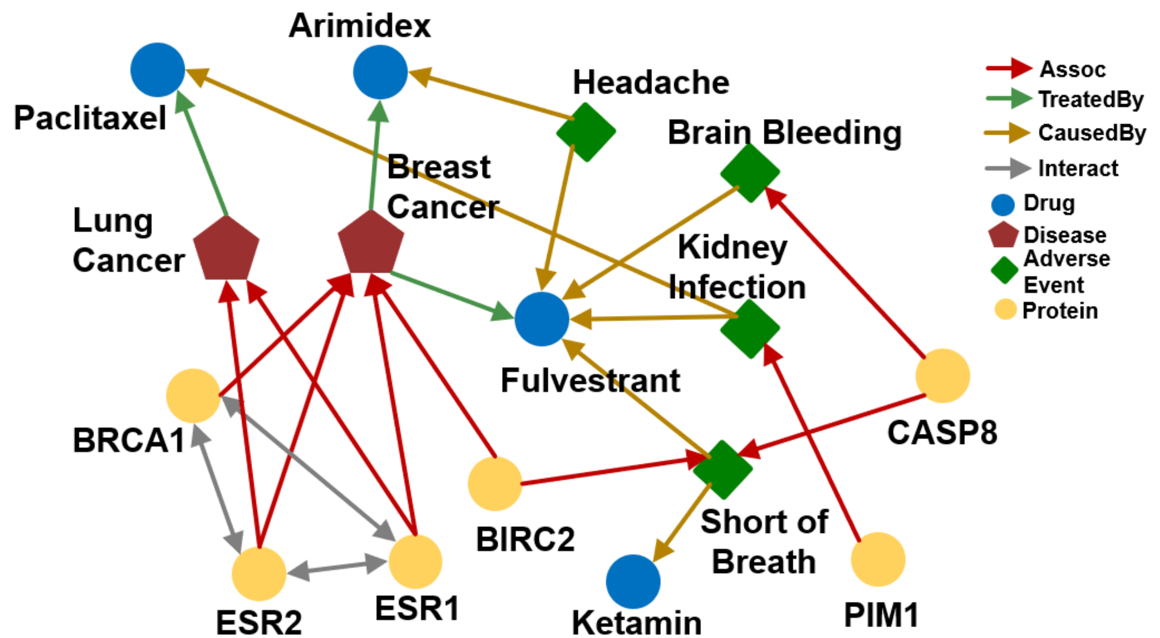


Conjunctive Queries

- *"What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?"*

((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))

How do we answer the question by KG traversal?

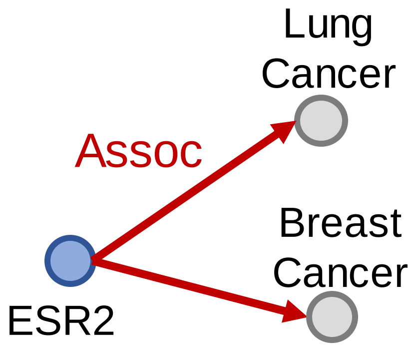


Traversing KG for Conjunctive Queries

- *"What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?"*

((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))

Traverse KG from **anchor nodes**: **ESR2** and **Short of Breath:**



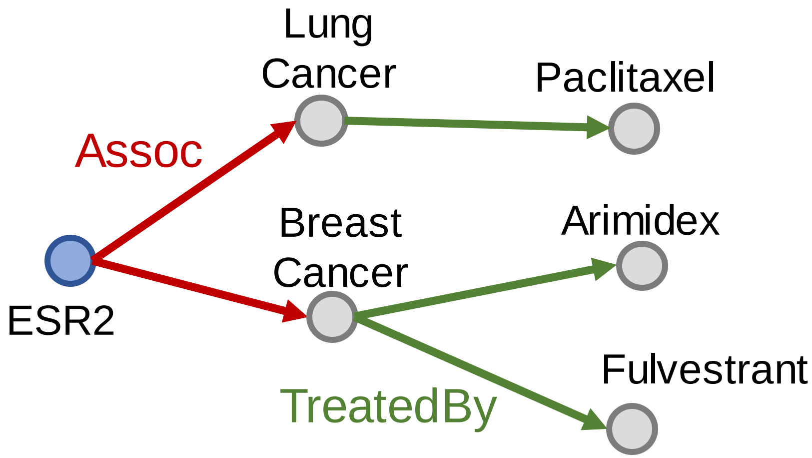
Traverse from the first anchor "ESR2" by relation "Assoc", we reach a set of entities {"Lung Cancer", "Breast Cancer"}

Traversing KG for Conjunctive Queries

- *"What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?"*

((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))

Traverse KG from **anchor nodes**: **ESR2** and **Short of Breath:**



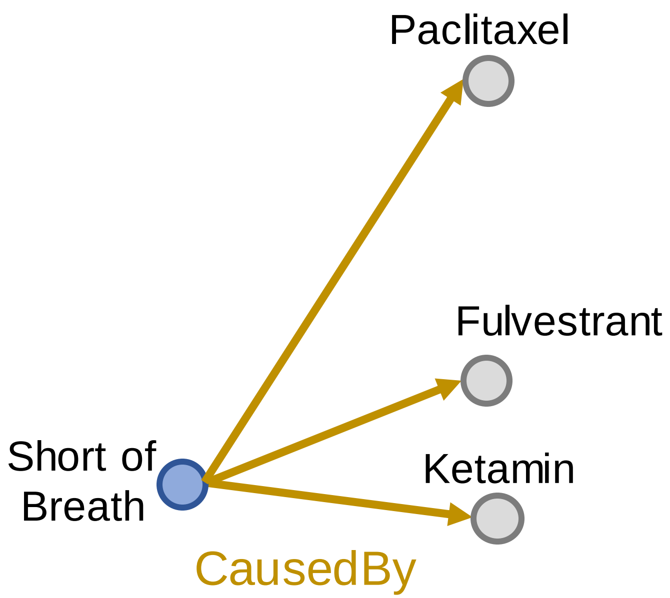
Traverse from the set of entities {"Lung Cancer", "Breast Cancer"} by relation TreatedBy, we reach a set of entities {"Paclitaxel", "Arimidex", "Fulvestrant"}

Traversing KG for Conjunctive Queries

- *"What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?"*

((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))

Traverse KG from **anchor nodes**: **ESR2** and **Short of Breath:**



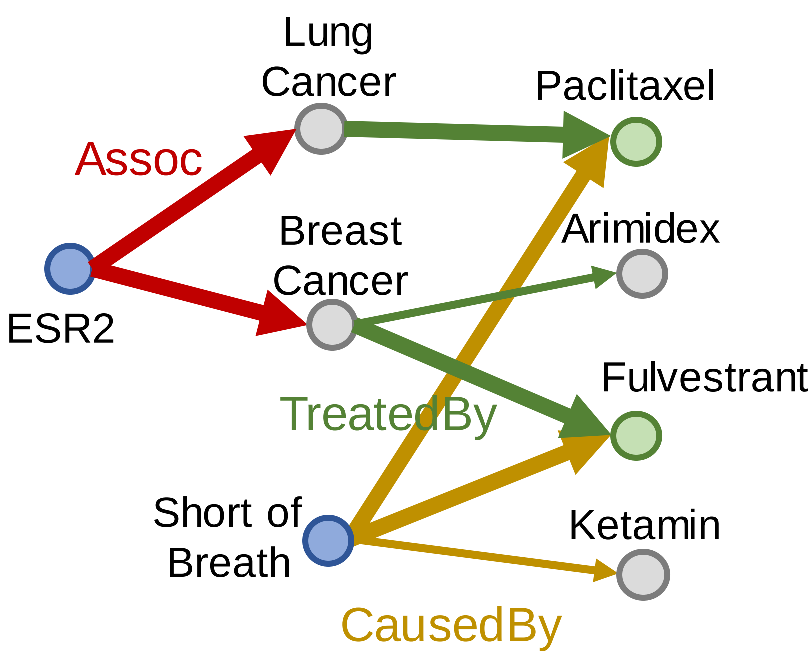
Traverse from the second anchor "Short of Breath" by relation "CausedBy", we reach a set of entities {"Fulvestrant", "Ketamin", "Paclitaxel"}

Traversing KG for Conjunctive Queries

- *"What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?"*

((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))

Traverse KG from **anchor nodes**: **ESR2** and **Short of Breath:**



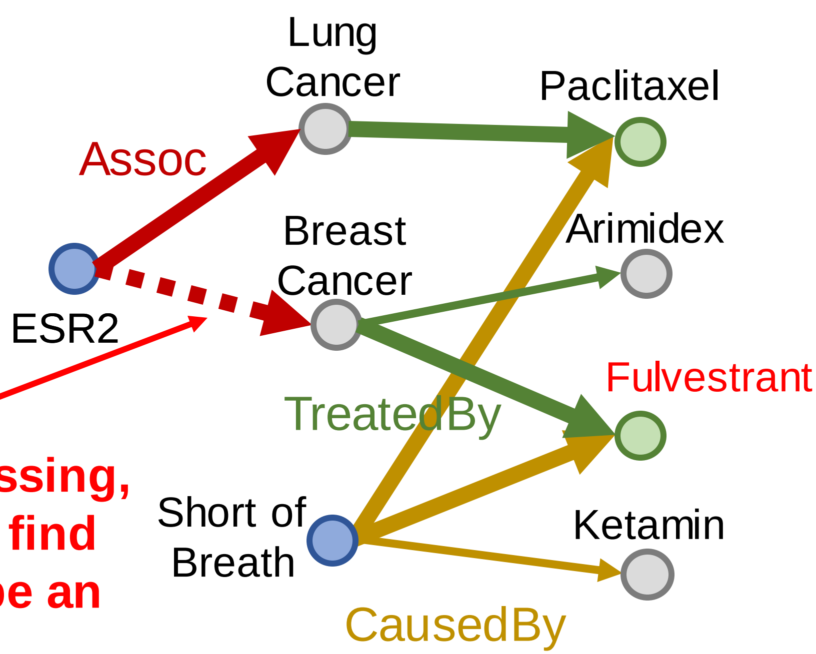
We take intersection between the two sets and get the answers {"Fulvestrant", "Paclitaxel"}

Traversing KG for Conjunctive Queries

- *"What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?"*

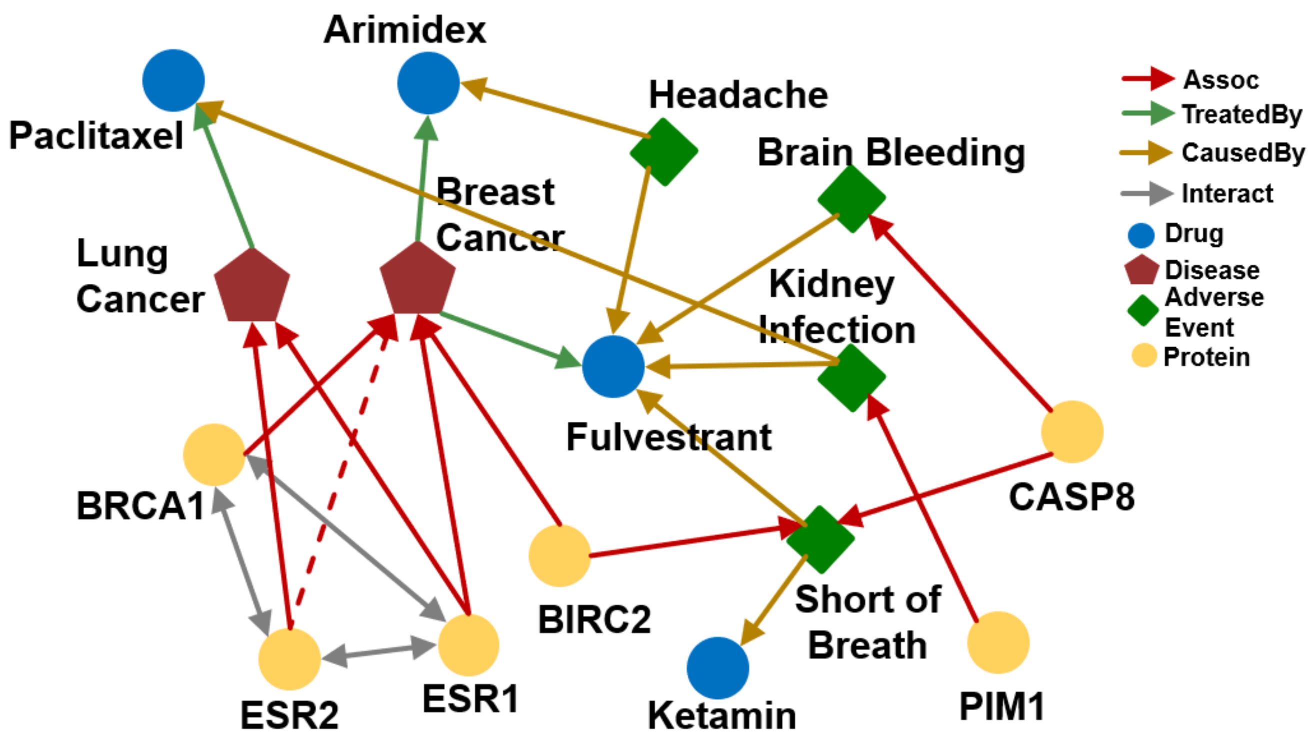
((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))

Traverse KG from **anchor nodes**: **ESR2** and **Short of Breath:**



If this link is missing, then we cannot find Fulvestrant to be an answer

Traversing KG for Conjunctive Queries



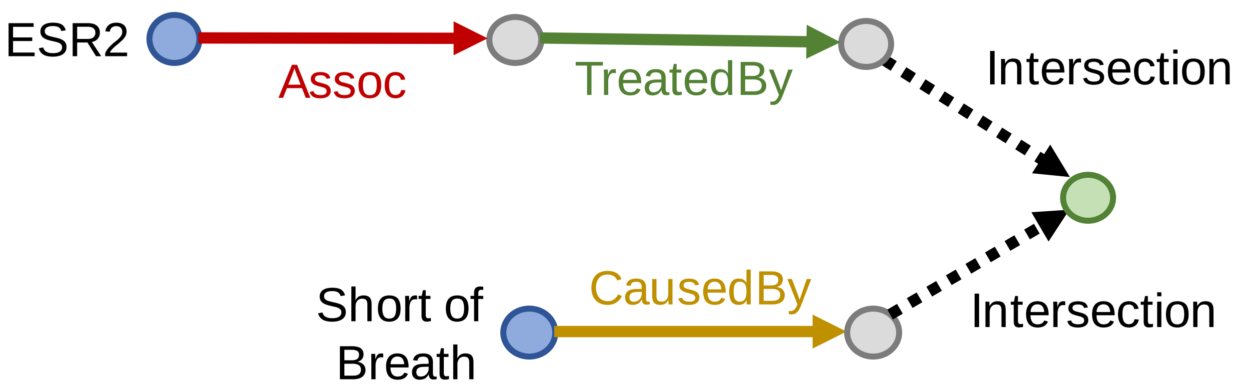
- How can we use embeddings to implicitly impute the **missing (ESR2, Assoc, Breast Cancer)?**
- **Intuition:** **ESR2** interacts with both **BRCA1** and **ESR1**. Both proteins are associated with **breast cancer**.

Traversing KG in Vector Space

- *"What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?"*

((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))

Query plan:



Each intermediate node represents a <u>set of entities</u>, how do we represent it? How do we define the intersection operation in the latent space?

Stanford CS224W: Query2Box: Reasoning over KGs Using Box Embeddings

CS224W: Machine Learning with Graphs

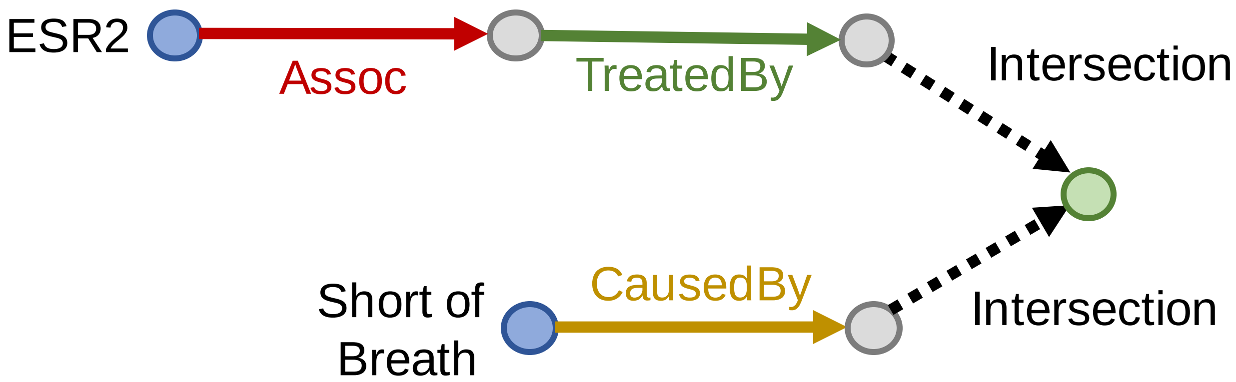
Jure Leskovec, Stanford University

http://cs224w.stanford.edu

Conjunctive Queries

How can we answer **more complex queries with logical conjunction operation**?

Query plan:



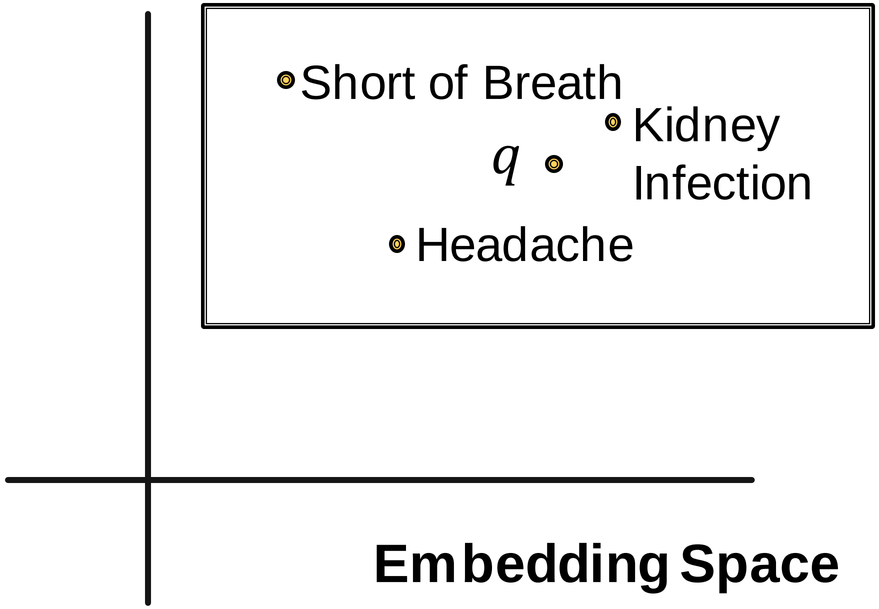
(1) Each intermediate node represents a set of entities; how do we represent it?

(2) How do we define the intersection operation in the latent space?

Box Embeddings

- Embed queries with **hyper-rectangles (boxes)**

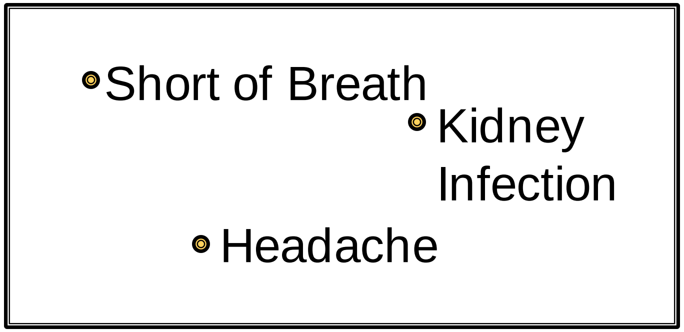
$$\mathbf{q} = (Center(q), Offset(q))$$



For example, we can embed the adverse events of Fulvestrant with **a box that enclose all the answer entities**.

Key Insight: Intersection

- **Intersection of boxes is well-defined!**
- When we traverse the KG to find the answers, each step produces a set of reachable entities.
- **How can we better model these sets?**
  - Boxes are a **powerful abstraction**, as we can project the center and control the offset to model the set of entities enclosed in the box



Embed with Box Embedding

Things to figure out:

- **Entity embeddings** (# params: $d|V|$):
  - Entities are seen as zero-volume boxes
- **Relation embeddings** (# params $2d|R|$)
  - Each relation takes a box and produces a new box
- **Intersection operator f :**
  - New operator, inputs are boxes and output is a box
  - Intuitively models intersection of boxes

Notation
d: out degree
|V|: # entities
|R|: # relations

Embed with Box Embedding

- **Embed queries in vector space:** *"What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?"*
  ((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))

Traverse KG from **anchor nodes**: **ESR2** and **Short of Breath:**

Query plan **Embedding Space**

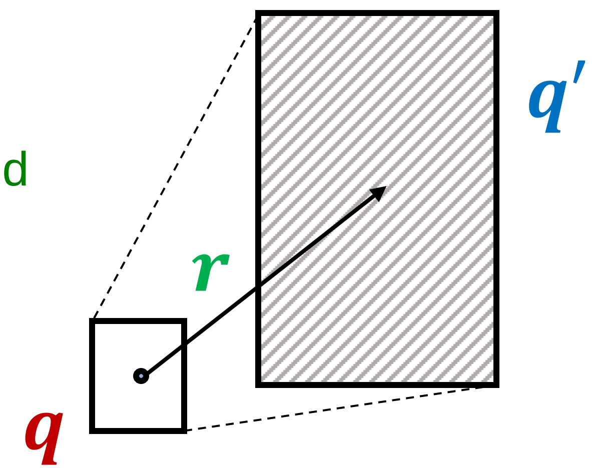
Projection Operator

Projection Operator $\mathcal{P}$

- **Intuition**:
  - Take the current box as input and use the relation embedding to **project and expand** the box!
- $\mathcal{P}$: Box × Relation → Box

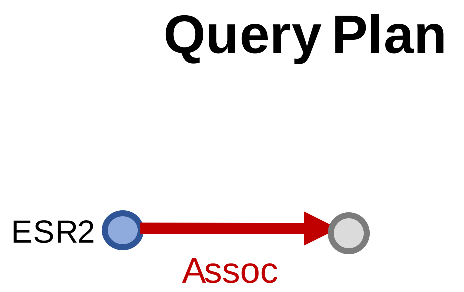
$$Cen(q') = Cen(q) + Cen(r)$$
$$Off(q') = Off(q) + Off(r)$$

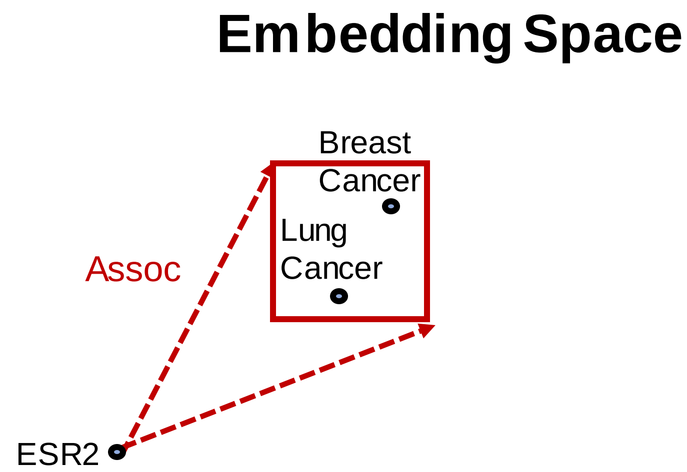
"×" (cross) means the projection operator is a **relation** from any box and **relation** to a new box



Embed with Box Embedding

- **Embed queries in vector space:** *"What are drugs that cause Short of Breath and treat diseases associated with protein ESR2?"*
- Traverse KG from **anchor nodes**: **ESR2** and **Short of Breath:**
- Use **projection operator** again following the query plan.





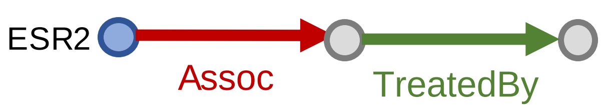
Embed with Box Embedding

"What is the drug that causes Short of Breath and treats disease associated with protein ESR2?"

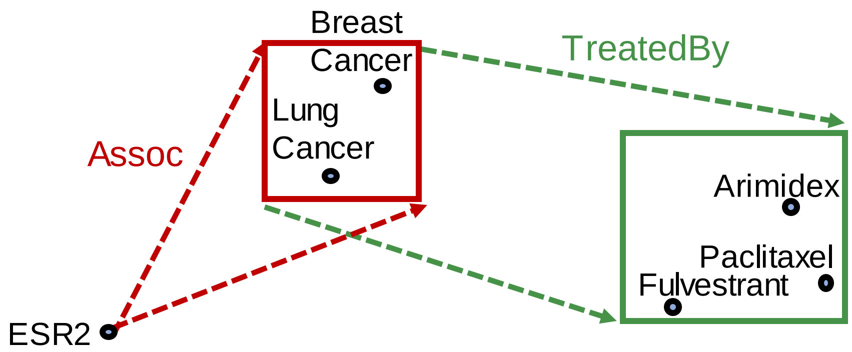
((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))

- Use **projection operator** again following the query plan.

Query Plan



Embedding Space



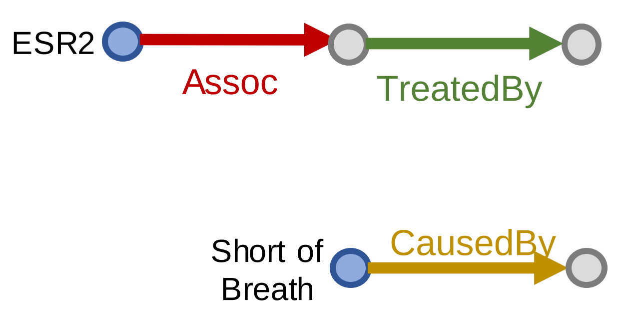
Embed with Box Embedding

"What is the drug that causes Short of Breath and treats disease associated with protein ESR2?"

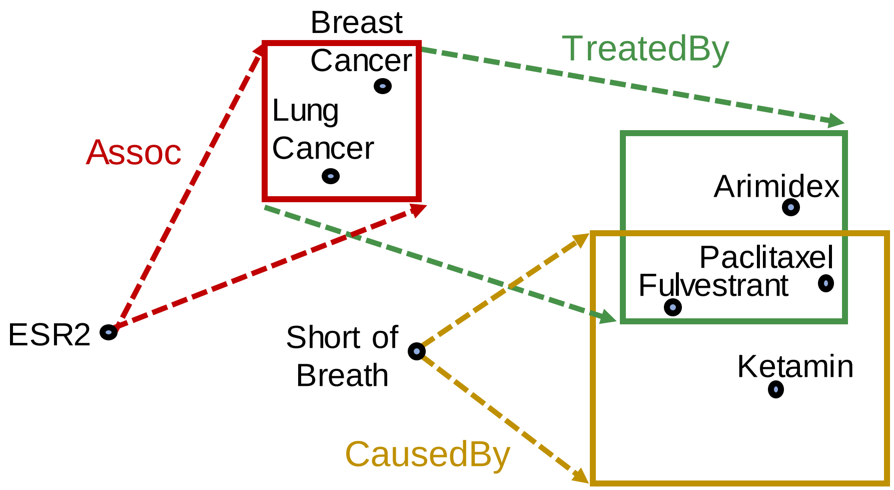
((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))

- Use **projection operator** again following the query plan.

Query Plan



Embedding Space

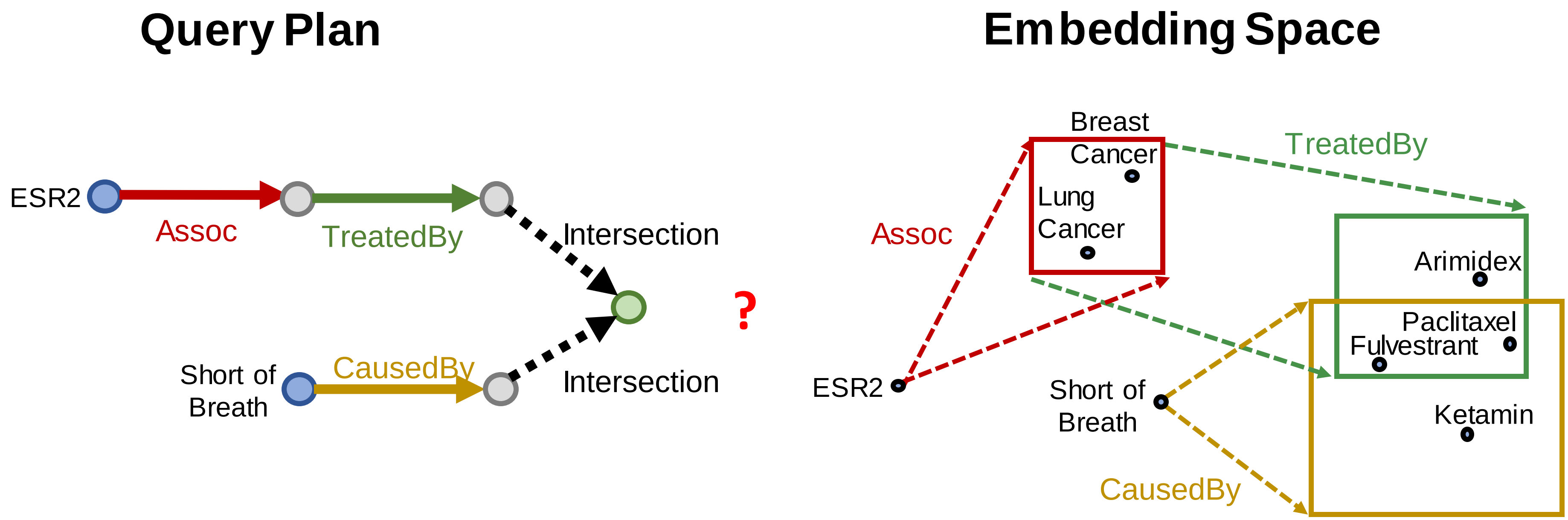


Embed with Box Embedding

"What is the drug that causes Short of Breath and treats disease associated with protein ESR2?"

((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))

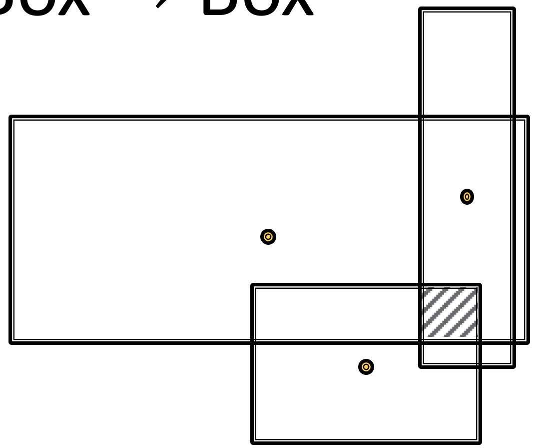
- **How do we take intersection of boxes?**



Intersection Operator

Geometric Intersection Operator $\mathcal{J}$

- Take multiple boxes as input and produce the intersection box
- **Intuition:**
  - The center of the new box should be **"close"** to the centers of the input boxes
  - The offset (box size) should **shrink** (since the size of the intersected set is **smaller** than the size of all the input set)
- $\mathcal{J}$: Box $\times \cdots \times$ Box $\rightarrow$ Box



Intersection Operator

Geometric Intersection Operator $\mathcal{J}$

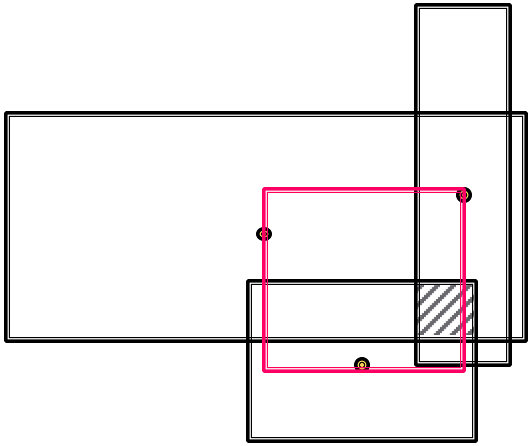
- $\mathcal{J}$: Box $\times \cdots \times$ Box $\rightarrow$ Box

Hadamard product
(element-wise product)

$$Cen(q_{inter}) = \sum_i \boldsymbol{w}_i \odot Cen(q_i)$$

$$\boldsymbol{w}_i = \frac{\exp(f_{cen}(Cen(q_i)))}{\sum_j \exp(f_{cen}(Cen(q_j)))}$$

$Cen(q_i) \in \mathbb{R}^d$
$\boldsymbol{w}_i \in \mathbb{R}^d$



Intuition: The center should be in the red region!
Implementation: The center is a **weighted sum** of the input box centers

$\boldsymbol{w}_i \in \mathbb{R}^d$ is calculated by a neural network f_{cen} (with trainable weights)
$\boldsymbol{w}_i$ **represents a "self-attention" score for the center of each input** $Cen(q_i)$.

Intersection Operator

Geometric Intersection Operator $\mathcal{J}$

- $\mathcal{J}$: Box × ⋯ × Box → Box

$$Off(q_{inter}) = \min\big(Off(q_1), \dots, Off(q_n)\big) \odot \sigma(f_{off}(Off(q_1), \dots, Off(q_n)))$$

guarantees shrinking

Sigmoid function: squashes output in (0,1)

f_{off} is a neural network (with trainable parameters) that extracts the representation of the input boxes to increase expressiveness

Intuition: The offset should be smaller than the offset of the input box

Implementation: We first **take minimum** of the offset of the input box, and then we make the model more expressive by introducing a new function f_{off} to extract the **representation** of the input boxes with a **sigmoid function** to **guarantee shrinking**.

Embed with Box Embedding

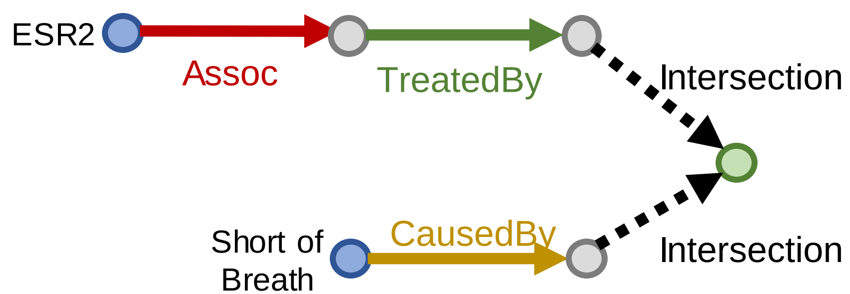
"What is the drug that causes Short of Breath and treats disease associated with protein ESR2?"

((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))

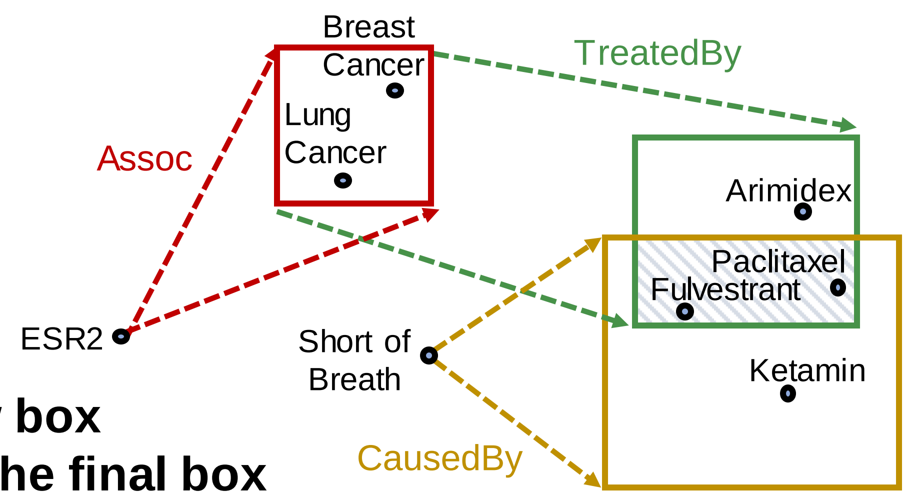
- **Use box intersection operator**

Summary: intersection operator, projection operators; box embeddings, anchor embeddings,

Query Plan



Embedding Space



The shadow box represents the final box embedding of the query

Entity-to-Box Distance

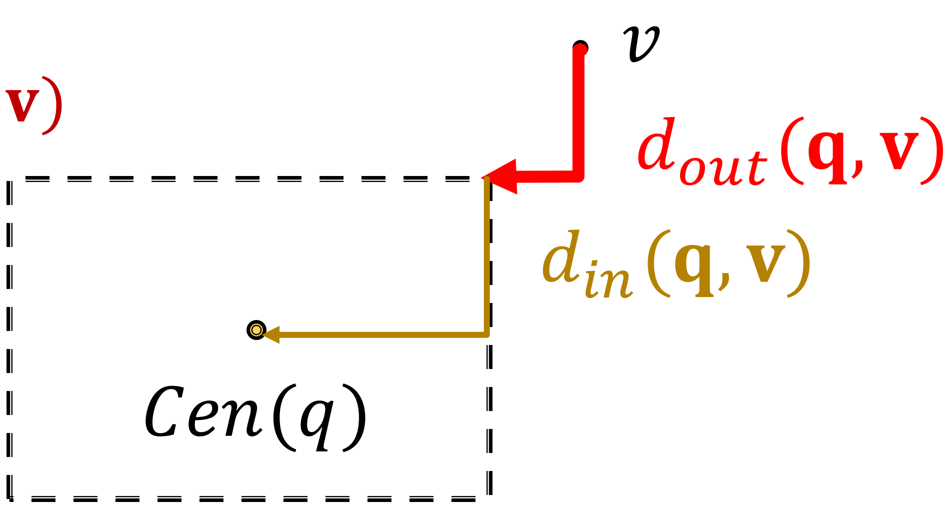
- **How do we define the score function $f_q(v)$ (negative distance)?**
  ($f_q(v)$ captures inverse distance of a node v as answer to q)
- Given a query box $\mathbf{q}$ and entity embedding (box) $\mathbf{v}$,

$$d_{box}(\mathbf{q}, \mathbf{v}) = d_{out}(\mathbf{q}, \mathbf{v}) + \alpha \cdot d_{in}(\mathbf{q}, \mathbf{v})$$

where $0 < \alpha < 1$.

- **Intuition**: if the point is enclosed in the box, the distance should be **downweighted**.
- $f_q(v) = -d_{box}(\mathbf{q}, \mathbf{v})$

Lost Function



Extending to Union Operation

- **Can we embed complex queries with union?**
  E.g.: "*What drug can treat breast cancer* ***or*** *lung cancer?*"

- **Conjunctive queries + disjunction** is called **E**xistential **P**ositive **F**irst-**o**rder (**EPFO**) queries. We'll refer to them as **AND-OR** queries.

- **Can we also design a disjunction operator and embed AND-OR queries in low-dimensional vector space?**

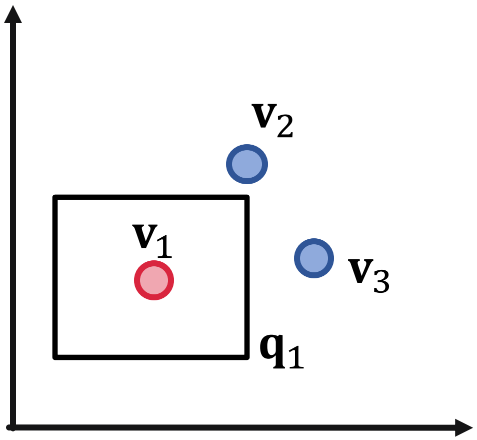
Embedding AND-OR Queries

- **Can we embed AND-OR queries in a low-dimensional vector space?**
- **No! Intuition**: Allowing **union** over **arbitrary queries** requires **high-dimensional** embeddings!

- **Example:**
  - Given 3 queries q_1, q_2, q_3, with answer sets:
  - $[\![q_1]\!] = \{v_1\}, [\![q_2]\!] = \{v_2\}, [\![q_3]\!] = \{v_3\}$
  - If we allow union operation, can we embed them in a **two-dimensional** plane?

Embedding AND-OR Queries

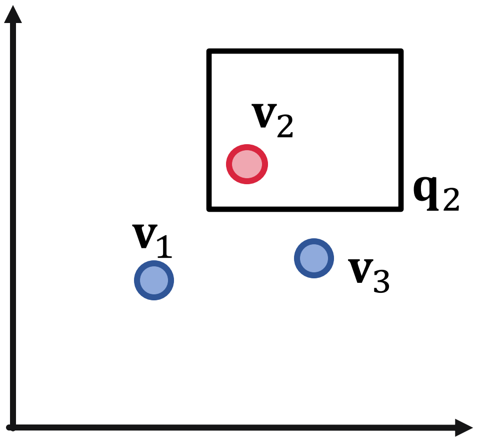
- **Example:**
  - Given 3 queries q_1, q_2, q_3, with answer sets:
  - $[\![q_1]\!] = \{v_1\}, [\![q_2]\!] = \{v_2\}, [\![q_3]\!] = \{v_3\}$
  - If we allow union operation, can we embed them in two-dimensional plane?



We want **red dots (answers)** to be in the box while the **blue dots (negative answers)** to be outside the box

Embedding AND-OR Queries

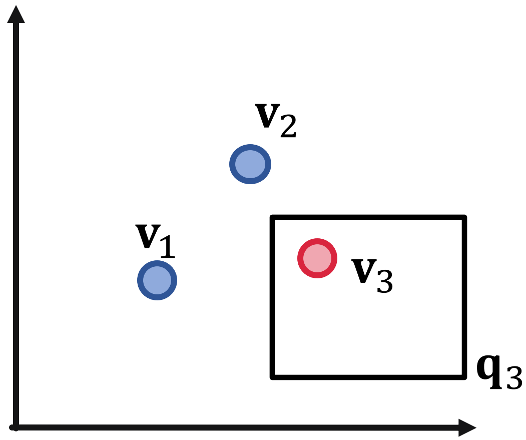
- **Example:**
  - Given 3 queries q_1, q_2, q_3, with answer sets:
  - $[\![q_1]\!] = \{v_1\}, [\![q_2]\!] = \{v_2\}, [\![q_3]\!] = \{v_3\}$
  - If we allow union operation, can we embed them in two-dimensional plane?



We want **red dots (answers)** to be in the box while the **blue dots (negative answers)** to be outside the box

Embedding AND-OR Queries

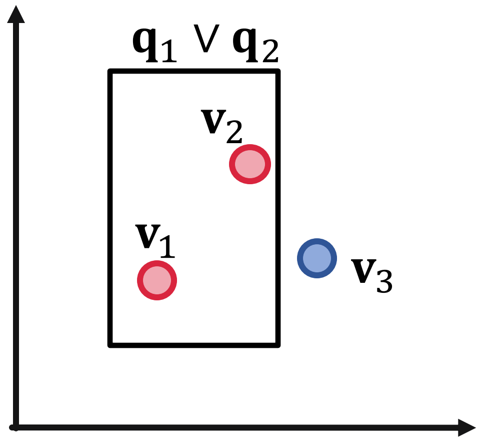
- **Example:**
  - Given 3 queries q_1, q_2, q_3, with answer sets:
  - $[\![q_1]\!] = \{v_1\}, [\![q_2]\!] = \{v_2\}, [\![q_3]\!] = \{v_3\}$
  - If we allow union operation, can we embed them in two-dimensional plane?



We want **red dots (answers)** to be in the box while the **blue dots (negative answers)** to be outside the box

Embedding AND-OR Queries

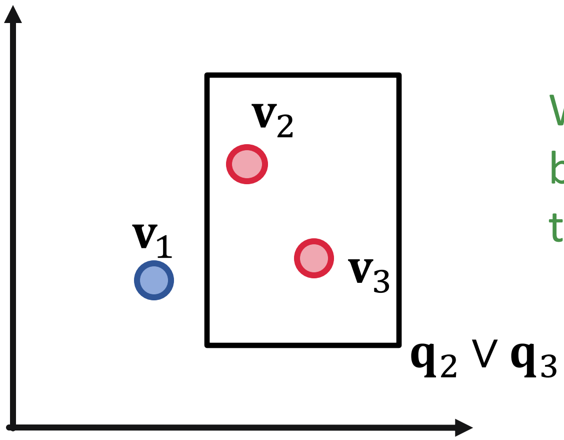
- **Example:**
  - Given 3 queries q_1, q_2, q_3, with answer sets:
  - $[\![q_1]\!] = \{v_1\}, [\![q_2]\!] = \{v_2\}, [\![q_3]\!] = \{v_3\}$
  - If we allow union operation, can we embed them in two-dimensional plane?



We want **red dots (answers)** to be in the box while the **blue dots (negative answers)** to be outside the box

Embedding AND-OR Queries

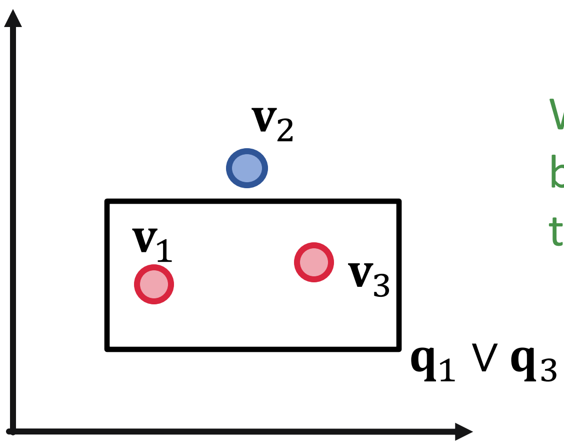
- **Example:**
  - Given 3 queries q_1, q_2, q_3, with answer sets:
  - $[\![q_1]\!] = \{v_1\}, [\![q_2]\!] = \{v_2\}, [\![q_3]\!] = \{v_3\}$
  - If we allow union operation, can we embed them in two-dimensional plane?



We want **red dots (answers)** to be in the box while the **blue dots (negative answers)** to be outside the box

Embedding AND-OR Queries

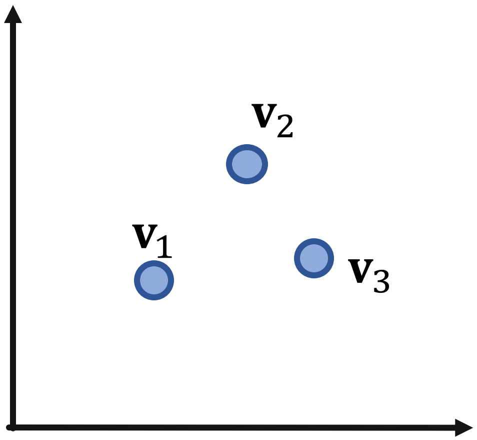
- **Example:**
  - Given 3 queries q_1, q_2, q_3, with answer sets:
  - $[\![q_1]\!] = \{v_1\}, [\![q_2]\!] = \{v_2\}, [\![q_3]\!] = \{v_3\}$
  - If we allow union operation, can we embed them in two-dimensional plane?



We want **red dots (answers)** to be in the box while the **blue dots (negative answers)** to be outside the box

Embedding AND-OR Queries

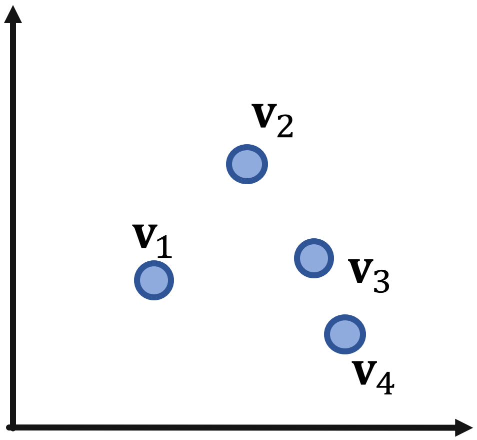
- **Example:**
  - Given 3 queries q_1, q_2, q_3, with answer sets:
  - $[\![q_1]\!] = \{v_1\}, [\![q_2]\!] = \{v_2\}, [\![q_3]\!] = \{v_3\}$
  - If we allow union operation, can we embed them in two-dimensional plane?



For 3 points, 2-dimension is okay!
How about 4 points?

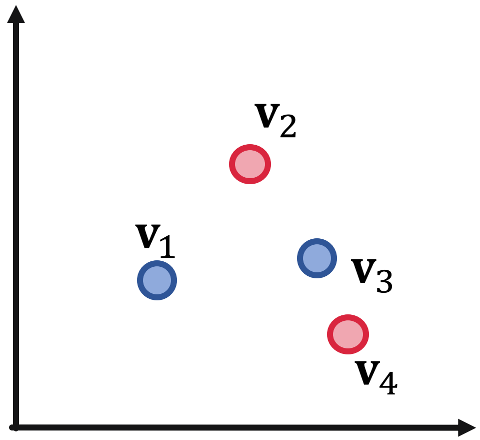
Embedding AND-OR Queries (2)

- **Example 2:**
  - Given 4 queries q_1, q_2, q_3, q_4 with answers:
  - $[\![q_1]\!] = \{v_1\}, [\![q_2]\!] = \{v_2\}, [\![q_3]\!] = \{v_3\}, [\![q_4]\!] = \{v_4\},$
  - If we allow union operation, can we embed them in two-dimensional plane?



Embedding AND-OR Queries (2)

- **Example 2:**
  - Given 4 queries q_1, q_2, q_3, q_4 with answers:
  - $[\![q_1]\!] = \{v_1\}, [\![q_2]\!] = \{v_2\}, [\![q_3]\!] = \{v_3\}, [\![q_4]\!] = \{v_4\},$
  - If we allow union operation, can we embed them in two-dimensional plane?



We cannot design a box embedding for $\boldsymbol{q_2} \vee \boldsymbol{q_4}$, that only v_2 and v_4 are in the box but v_1 and v_3 are outside the box.

Embedding AND-OR Queries (2)

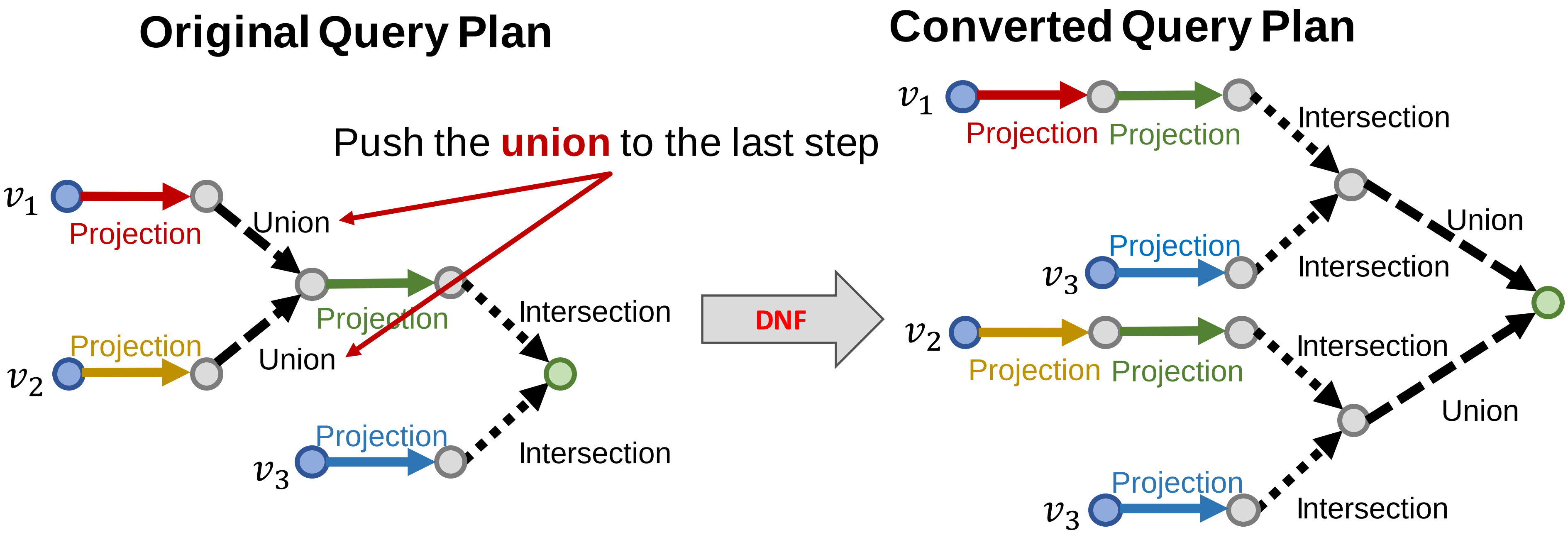
Can we embed AND-OR queries in low-dimensional vector space?

- **Conclusion**: Given any M conjunctive queries $q_1, \dots, q_M$ with non-overlapping answers, we need dimensionality of $\Theta(M)$ to handle all OR queries.
  - For real-world KG, such as FB15k, we find $M \geq 13{,}365$, where $|V| = 14{,}951$.
  - Remember, this is for arbitrary OR queries.

Embedding AND-OR Queries (3)

Since we **cannot embed** AND-OR queries in low-dimensional space, can we still handle them?

- **Key idea:** take all unions out and only do union **at the last step**!



Disjunctive Normal Form

- Any **AND-OR query** can be transformed into equivalent DNF, i.e., **disjunction of conjunctive queries**.

- **Given any AND-OR query q,**

$$q = q_1 \vee q_2 \vee \cdots \vee q_m$$

where q_i is a **conjunctive query**.

- Now we can first embed each q_i and then "**aggregate**" at the last step!

Distance Between q and an Entity

- **Distance** between entity embedding and a DNF $q = q_1 \vee q_2 \vee \cdots \vee q_m$ is defined as:

$$d_{box}(\mathbf{q}, \mathbf{v}) = min(d_{box}(\mathbf{q}_1, \mathbf{v}), \ldots, d_{box}(\mathbf{q}_m, \mathbf{v}))$$

- **Intuition:**
  - As long as v is the answer to one conjunctive query q_i, then v should be the answer to q
  - As long as $\mathbf{v}$ is close to one conjunctive query $\mathbf{q}_i$, then $\mathbf{v}$ should be close to $\mathbf{q}$ **in the embedding space**

Distance Between q and an Entity

- **Distance** between entity embedding and a DNF $q = q_1 \vee q_2 \vee \cdots \vee q_m$ is defined as:

$$d_{box}(\mathbf{q}, \mathbf{v}) = min(d_{box}(\mathbf{q}_1, \mathbf{v}), \ldots, d_{box}(\mathbf{q}_m, \mathbf{v}))$$

- **The process of embedding any AND-OR query q**
  1. Transform q to **equivalent DNF** $q_1 \vee \cdots \vee q_m$
  2. **Embed** q_1 to q_m
  3. Calculate the (box) distance $d_{box}(\mathbf{q}_i, \mathbf{v})$
  4. Take the **minimum** of all distance
  5. **The final score** $f_q(v) = -d_{box}(\mathbf{q}, \mathbf{v})$

Stanford CS224W: How to Train Query2box

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

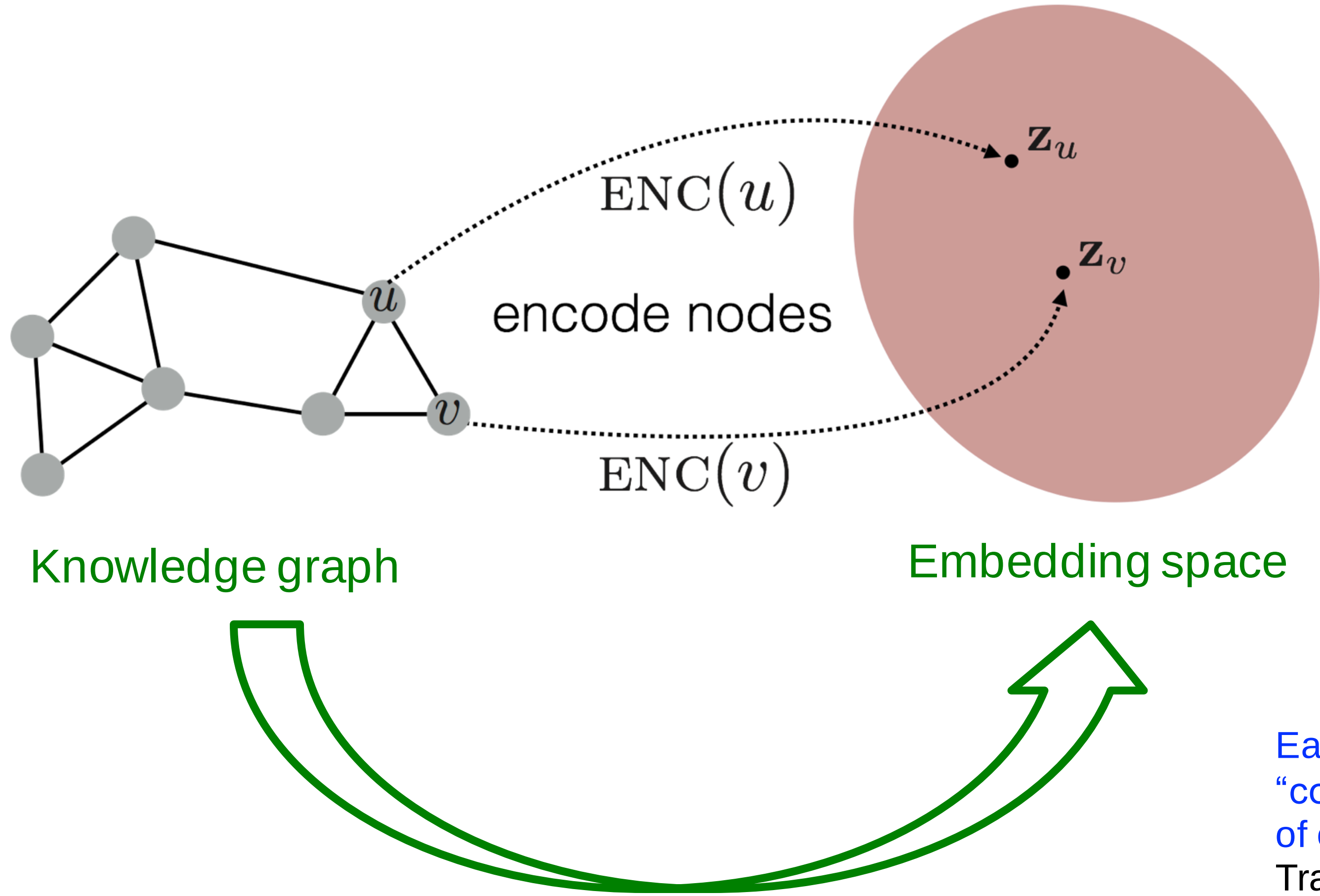
Training Overview

- **Overview and Intuition** (similar to KG completion):
  - Given a query embedding $\mathbf{q}$, maximize the score $f_q(v)$ for answers $v \in [\![q]\!]$ and minimize the score $f_q(v')$ for negative answers $v' \notin [\![q]\!]$
- Trainable parameters:
  - Entity embeddings with $d|V|$ # params
  - Relation embeddings with $2d|R|$ # params
  - Intersection operator
- **How to achieve a query, its answers, its negative answers from the KG to train the parameters?**
- **How to split the KG for query answering?**

Training Overview

(user specified)
Predictive query

Reason in the embedding space



Generate a set of training queries (q, v, v').
Train entity embeddings and operators to minimize the loss (i.e., to answer the training queries correctly).

Each training query provides a "constrain" on the embeddings of entities.

Training loop:

1) Get query (q, v, v')
2) Using current operators, embed q.
3) Compute the loss to update entity embs. and operators

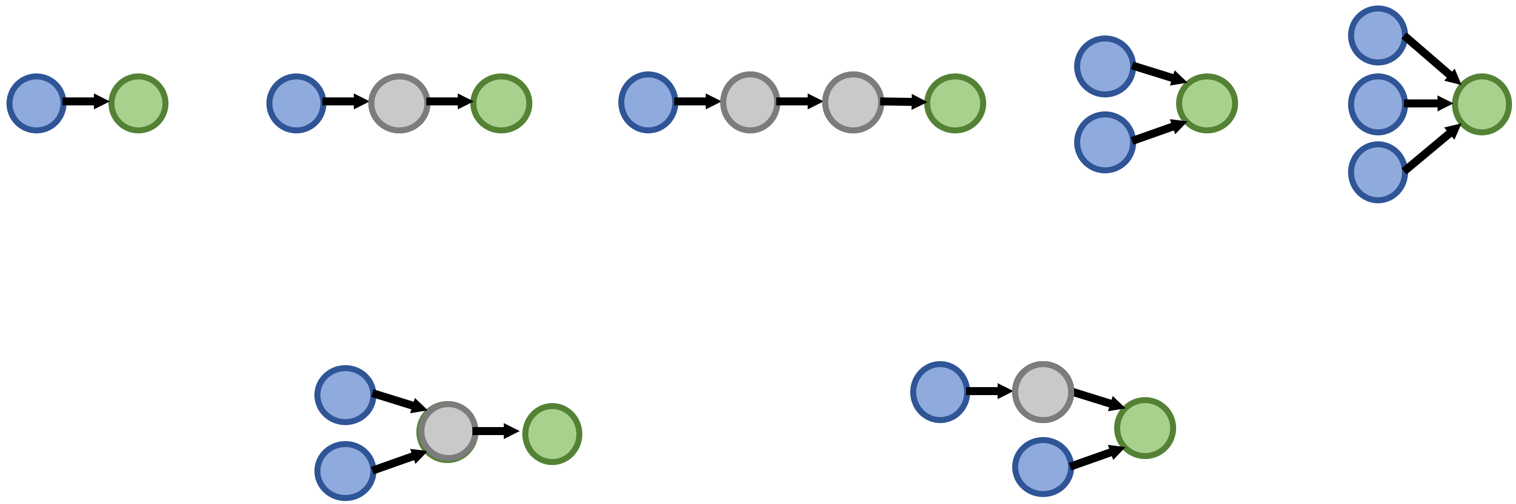
Training: Details

- **Training**:
  1. Sample a query q from the training graph G_{train}, answer $v \in [\![q]\!]_{G_{train}}$, and non-answer $v' \notin [\![q]\!]_{G_{train}}$
  2. Embed the query $\mathbf{q}$.
     - Use current operators, to compute query embedding.
  3. Calculate the score $f_q(v)$ and $f_q(v')$.
  4. Optimize embeddings and operators to minimize the loss ℓ (maximize $f_q(v)$ while minimize $f_q(v')$):

$$\ell = -\log \sigma\left(f_q(v)\right) - \log(1 - \sigma(f_q(v')))$$

Query Generation from Templates

- **Generate queries from multiple query templates:**

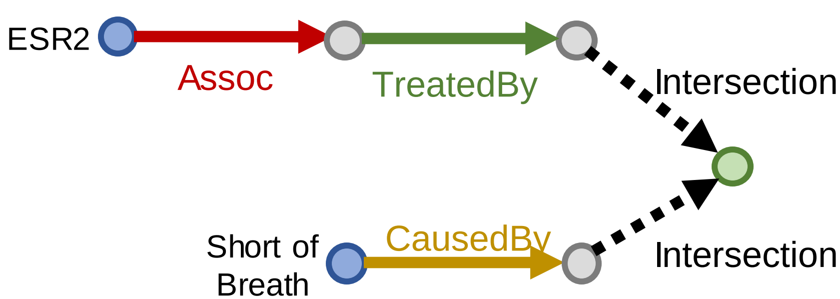


Query Generation from Templates

- How can we generate **a complex query**?
- We start with a **query template**
- **Query template** is an abstraction of the query
- We generate a query by instantiating every variable with a concrete entity and relation from the KG
  - E.g., instantiate **Anchor1** with **ESR2** (a node on KG)
  - E.g., instantiate **Rel1** with **Assoc** (an edge on KG)
- **How to instantiate query template given a KG?**

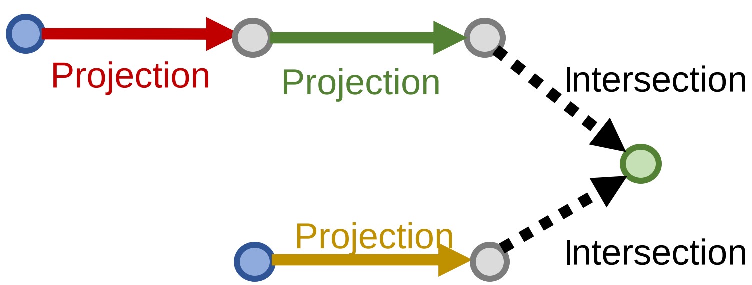
Query

((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))



Query Template

((Anchor1, (Rel1, Rel2)), (Anchor2, (Rel3))

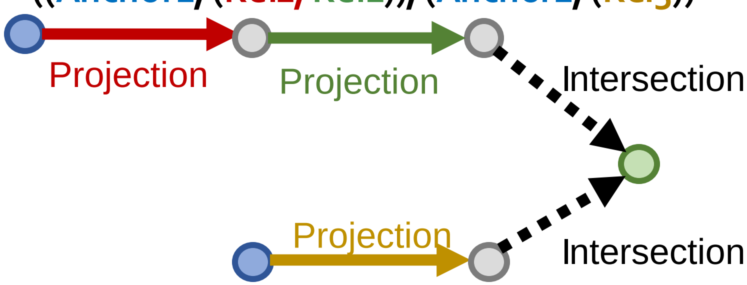


Query Generation from Templates

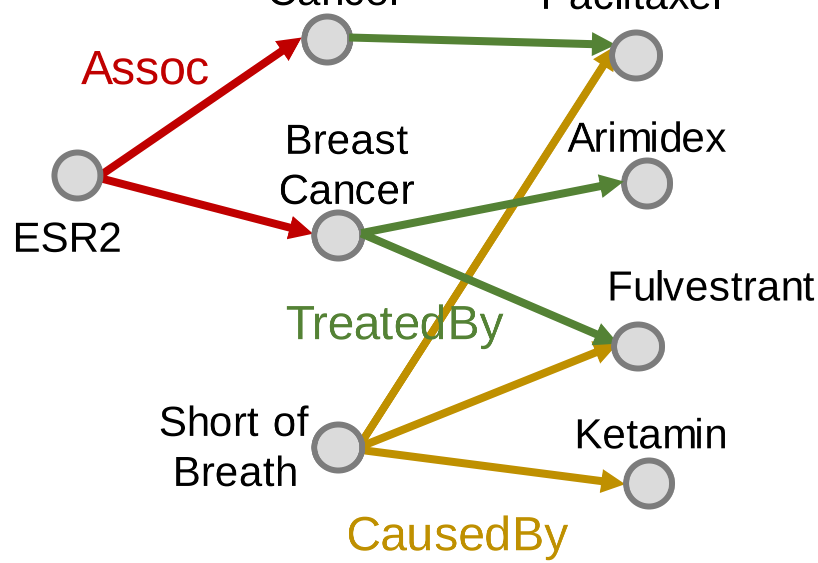
- **How to instantiate a query template given a KG?**

Query Template

((Anchor1, (Rel1, Rel2)), (Anchor2, (Rel3))



Knowledge Graph



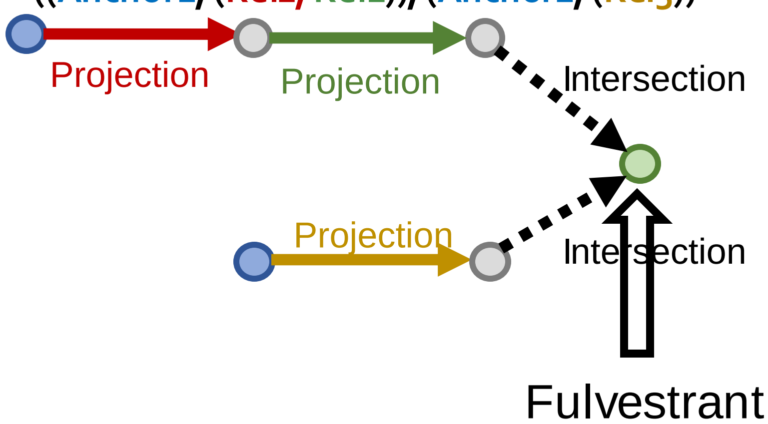
Overview:
Start from instantiating the **answer node** of the query template and then iteratively instantiate the other edges and nodes until we ground **all the anchor nodes**

Query Generation from Templates

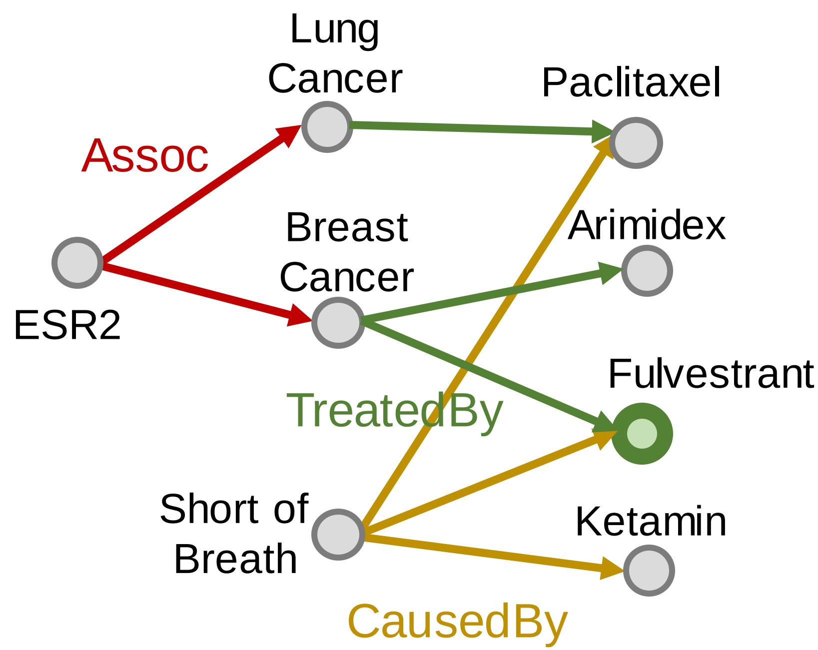
- **How to instantiate a query template given a KG?**

Query Template

((Anchor1, (Rel1, Rel2)), (Anchor2, (Rel3))



Knowledge Graph

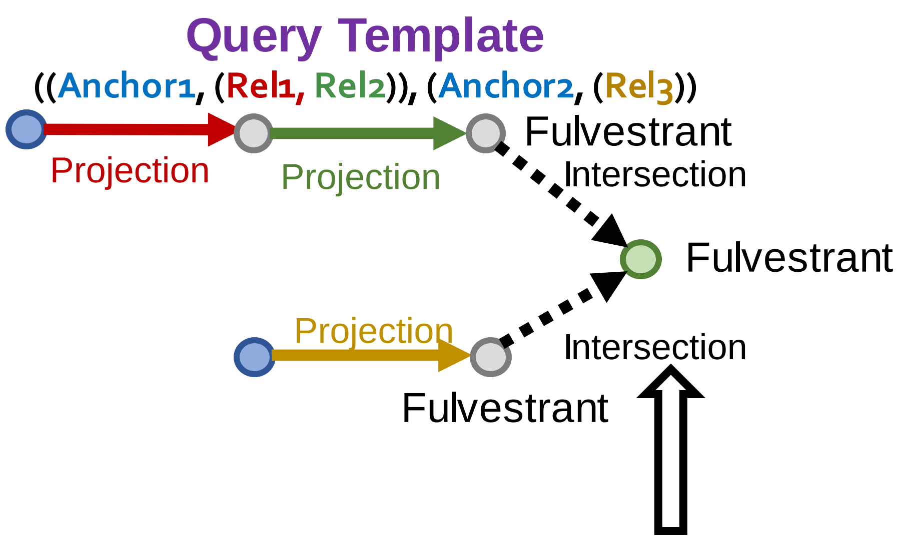


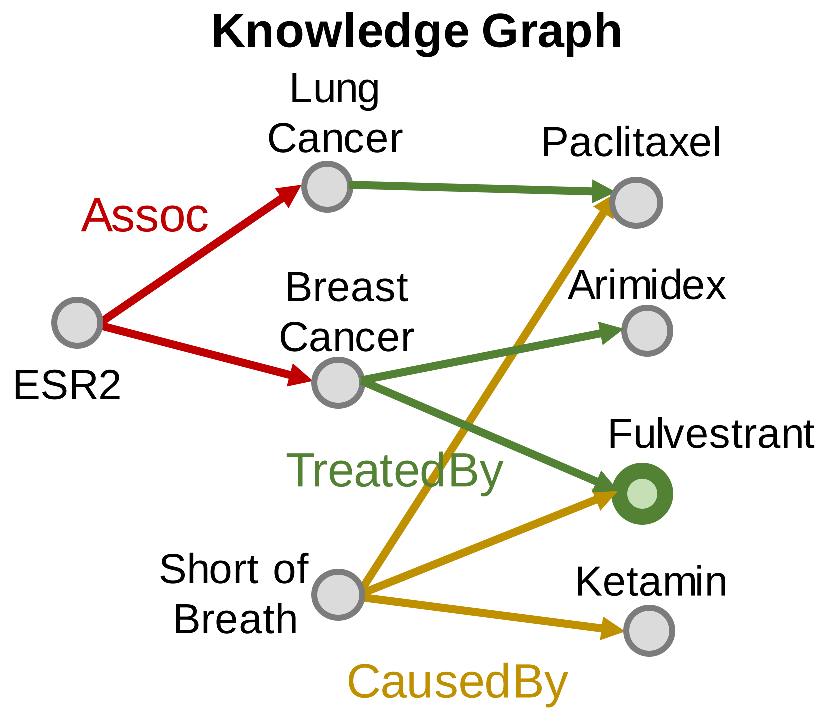
Start from instantiating the **root node** of the query template.

Randomly pick one entity from KG as the root node, e.g., we pick **Fulvestrant**.

Query Generation from Templates

- **How to instantiate a query template given a KG?**





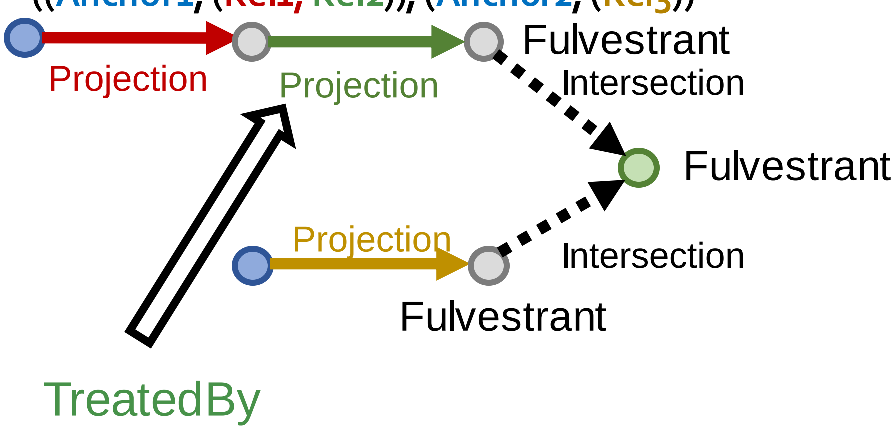
Now we look at intersection. What we have is that the intersection of the sets of entities is **Fulvestrant**, then naturally the two sets should also contain **Fulvestrant**.

Query Generation from Templates

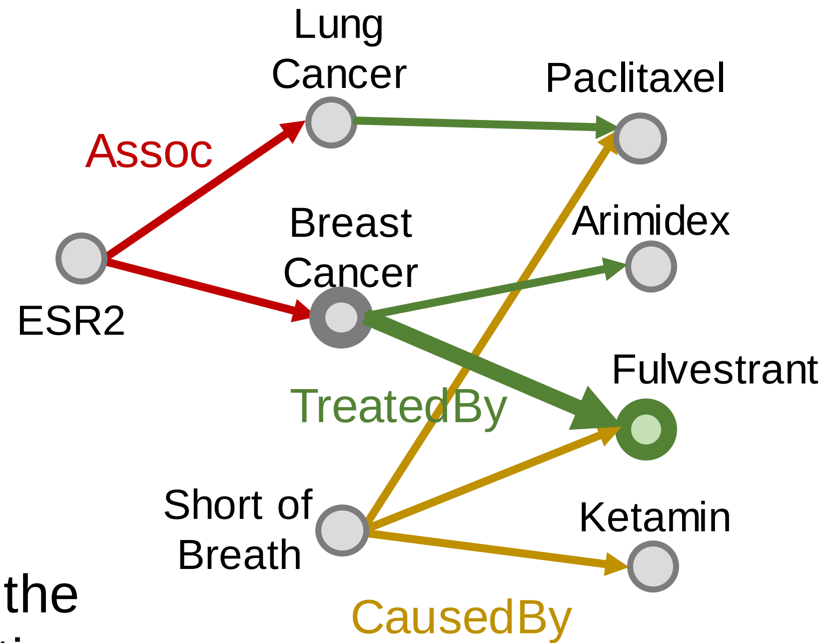
- **How to instantiate a query template given a KG?**

Query Template

((Anchor$_1$, (Rel$_1$, Rel$_2$)), (Anchor$_2$, (Rel$_3$)))



Knowledge Graph



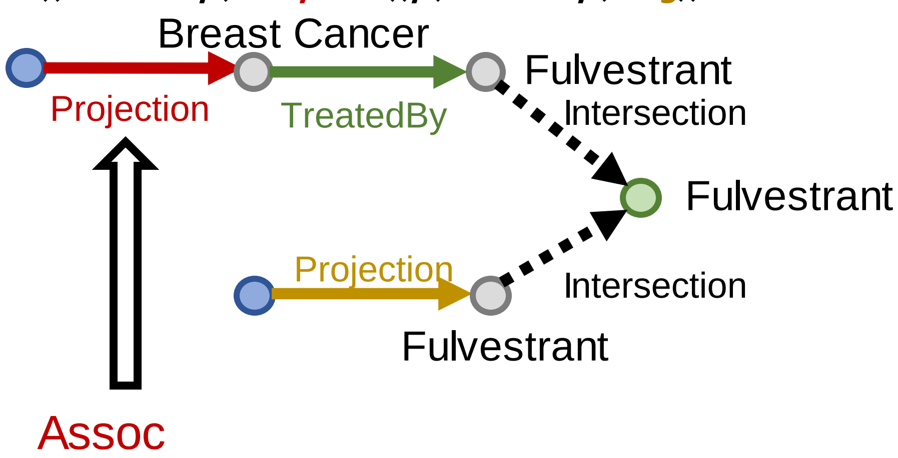
We instantiate the **Projection edge** in the template by randomly sample one relation associated with the current entity **Fulvestrant**. For example, we may select relation **TreatedBy**, and check what entities are connected to **Fulvestrant** with **TreatedBy**: {**Breast Cancer**}.

Query Generation from Templates

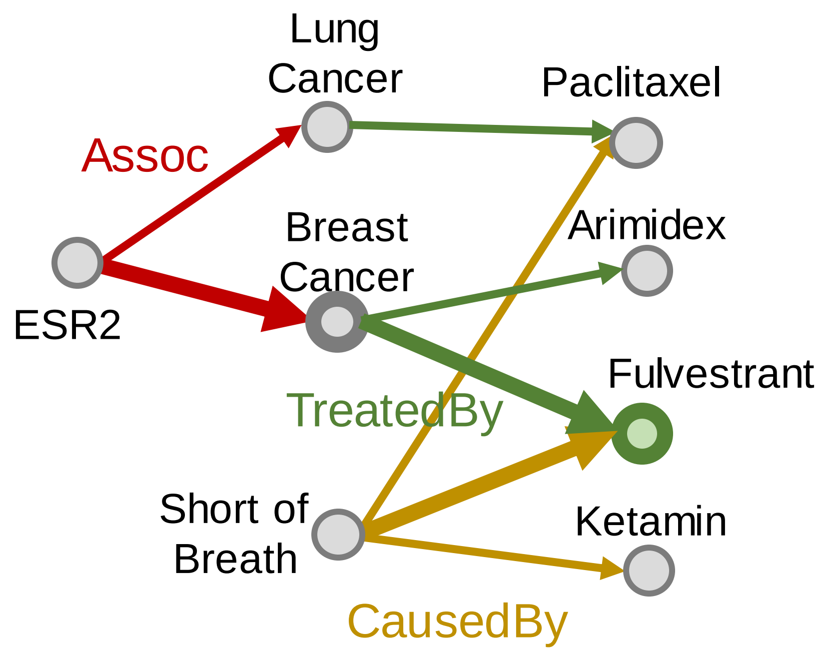
- **How to instantiate a query template given a KG?**

Query Template

((Anchor1, (Rel1, Rel2)), (Anchor2, (Rel3)))



Knowledge Graph



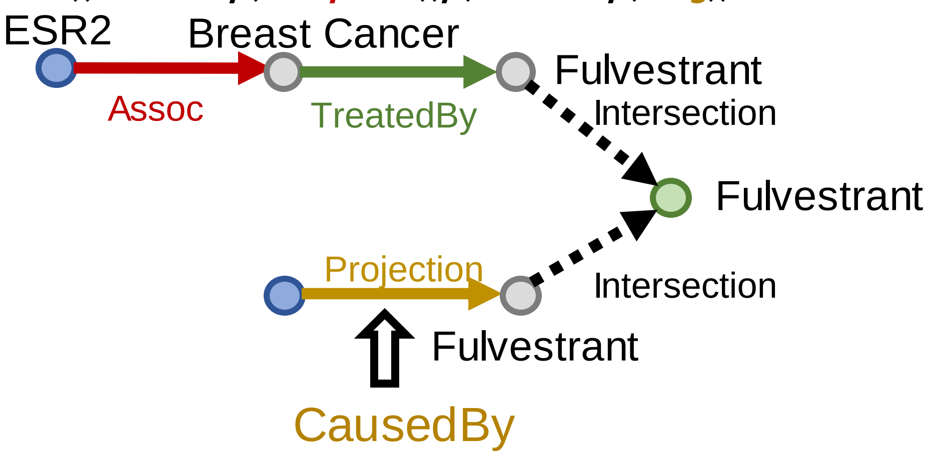
We first look at one branch and ground the **Projection edge** with the relation associated with **Breast Cancer**, e.g., **Assoc**. Then we check what entities are connected to **Breast Cancer** with **Assoc**: {**ESR2**}.

Query Generation from Templates

- **How to instantiate a query template given a KG?**

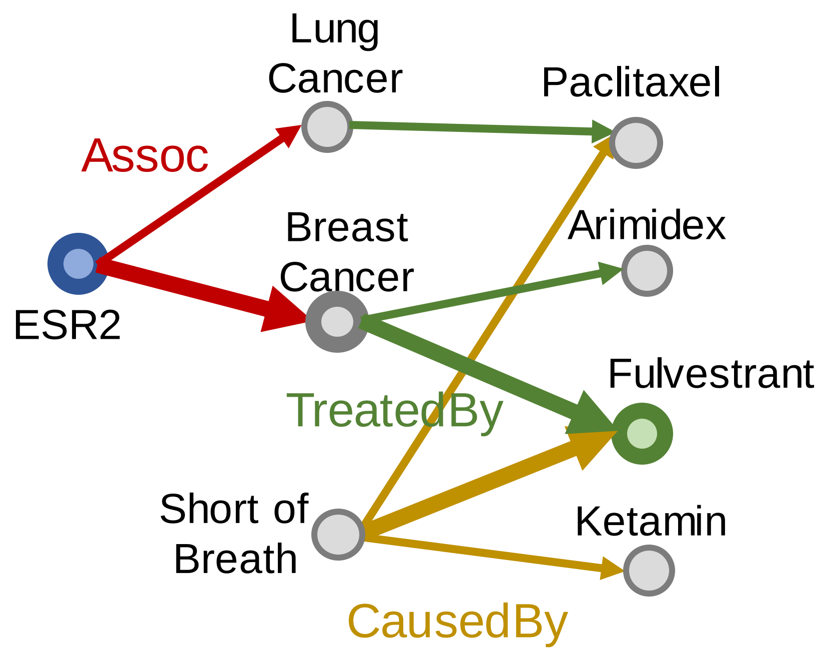
Query Template

((**Anchor1**, (**Rel1**, **Rel2**)), (**Anchor2**, (**Rel3**))



Then we look at the second branch and ground the **Projection edge** with the relation associated with **Fulvestrant**, e.g., **CausedBy**. Then we check what entities are connected to **Fulvestrant** with **CausedBy**: {**Short of Breath**}.

Knowledge Graph

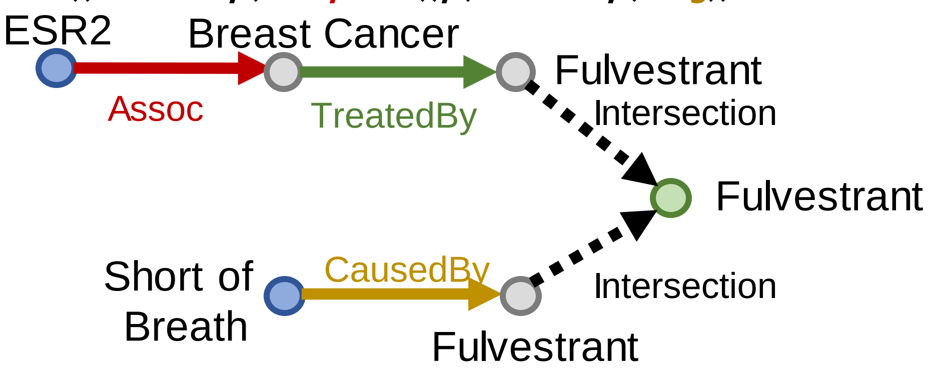


Query Generation from Templates

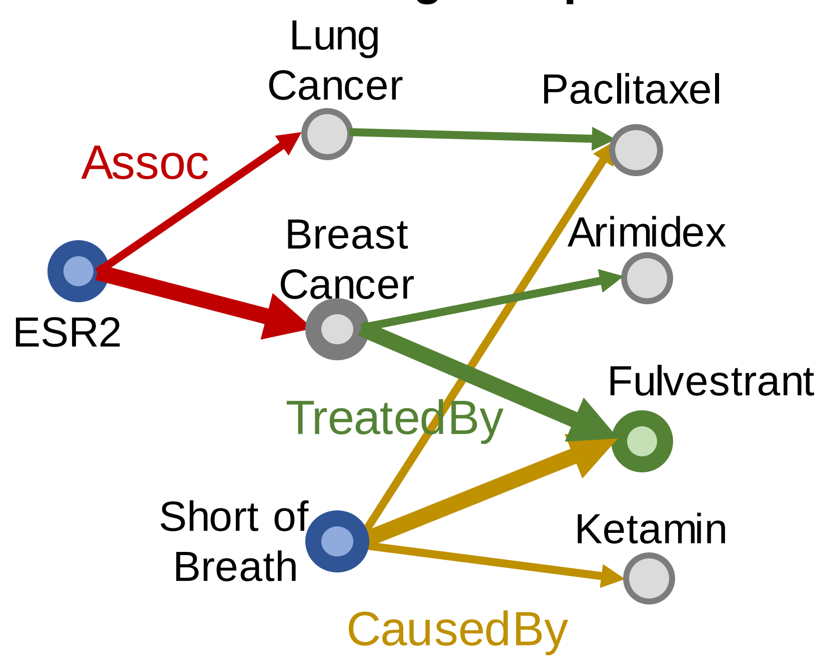
- **How to instantiate a query template given a KG?**

Query Template

((Anchor1, (Rel1, Rel2)), (Anchor2, (Rel3)))



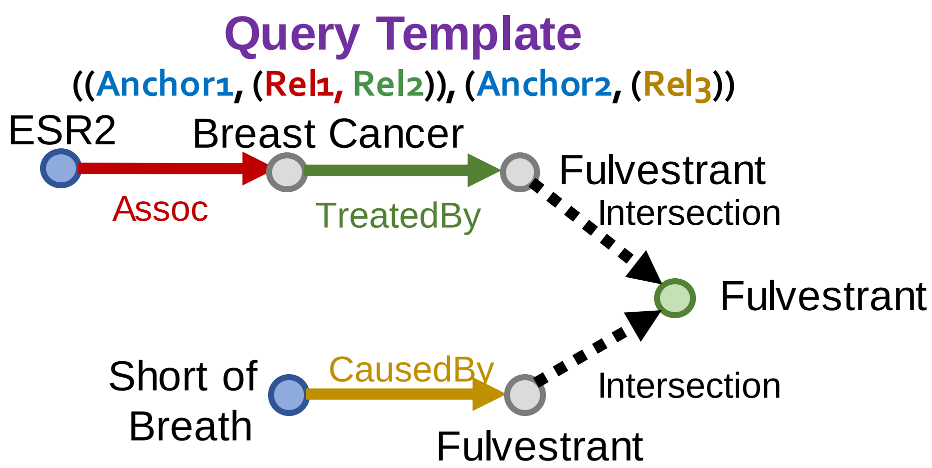
Knowledge Graph



We select entity from {**Short of Breath**}, set it as the anchor node.

Query Generation from Templates

- **How to instantiate a query template given a KG?**



Now, we instantiated a **query q**!

q: ((**e:ESR2**, (**r:Assoc**, **r:TreatedBy**)), (**e:Short of Breath**, (**r:CausedBy**))

- The query q **must** have answers on the KG and one of the answers is the instantiated answer node: **Fulvestrant**.
- We may obtain the full set of answers $[\![q]\!]_G$ by **KG traversal**.
- We can sample negative answers $v' \notin [\![q]\!]_G$

Stanford CS224W: Example of Query2box

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

http://cs224w.stanford.edu

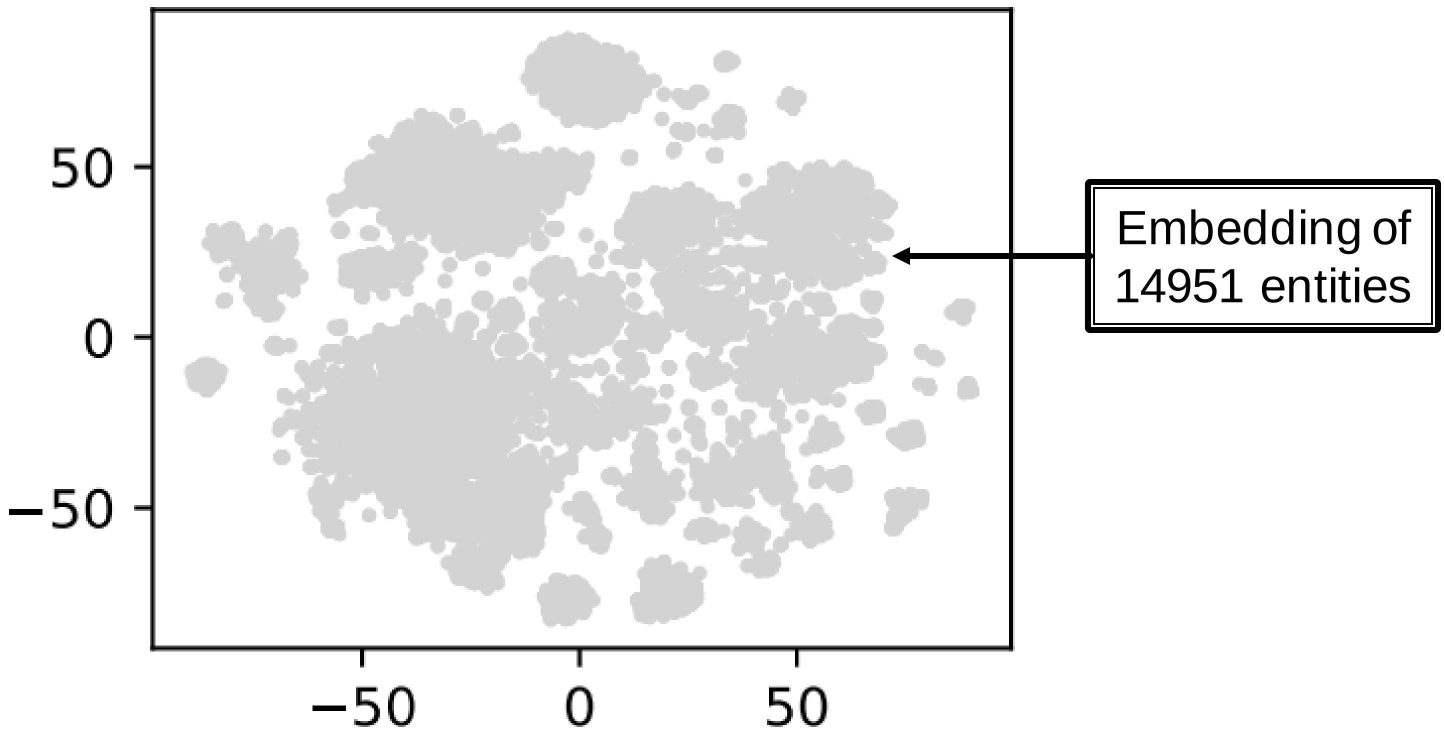
Visualization

- **What do box embeddings actually learn?**

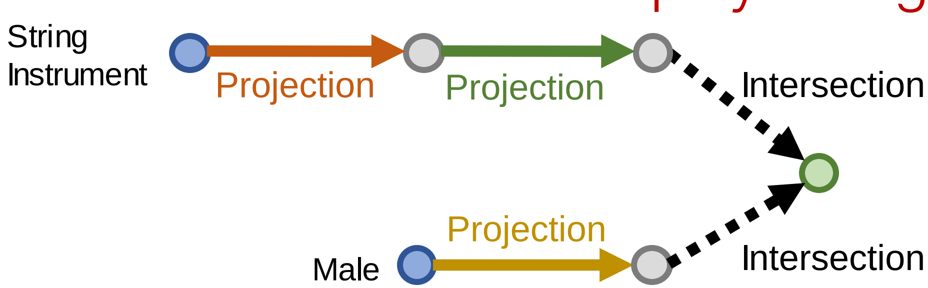
Example: "*List male instrumentalists who play string instruments*"

- We use t-SNE to reduce the embedding space to a 2-dimensional space, in order to visualize the query results

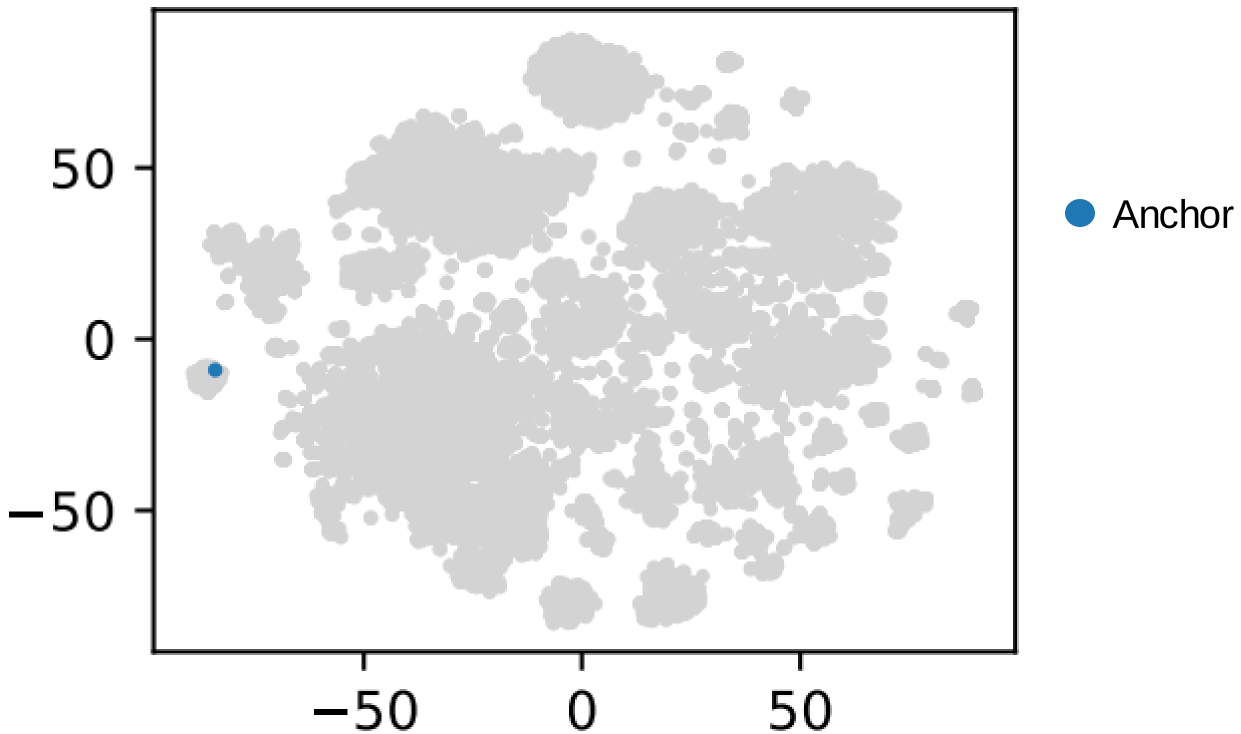
Embedding Space



"List male instrumentalists who play string instruments"

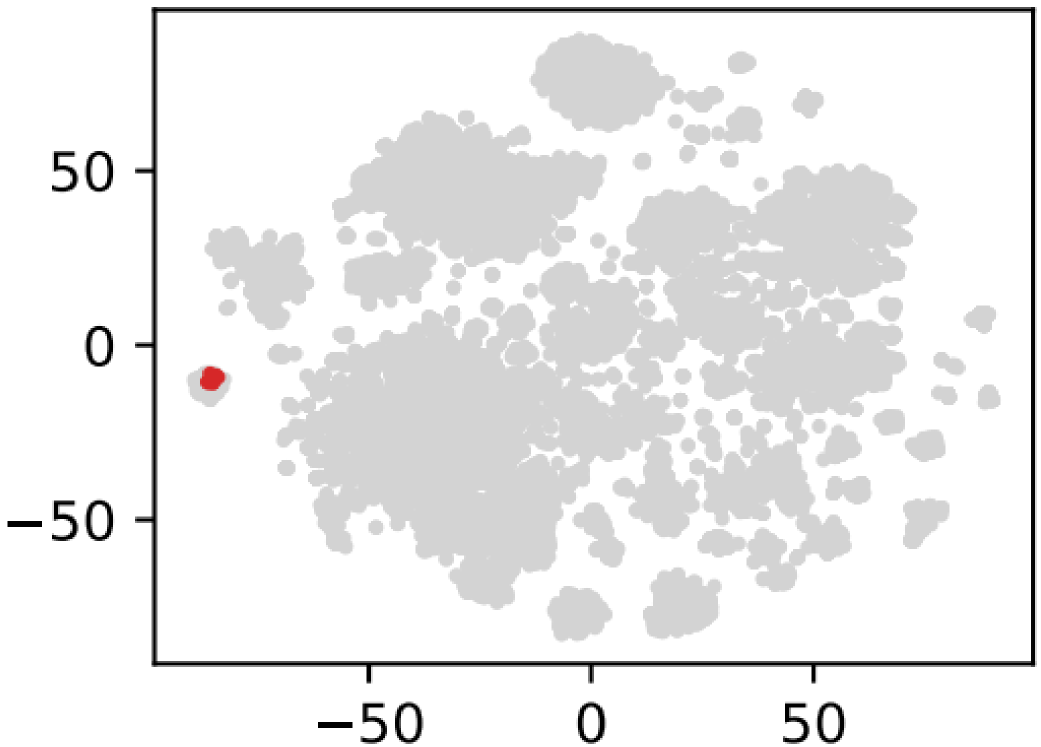


Embedding Space



“List male instrumentalists who play string instruments”

Embedding Space



# of string instruments: 10

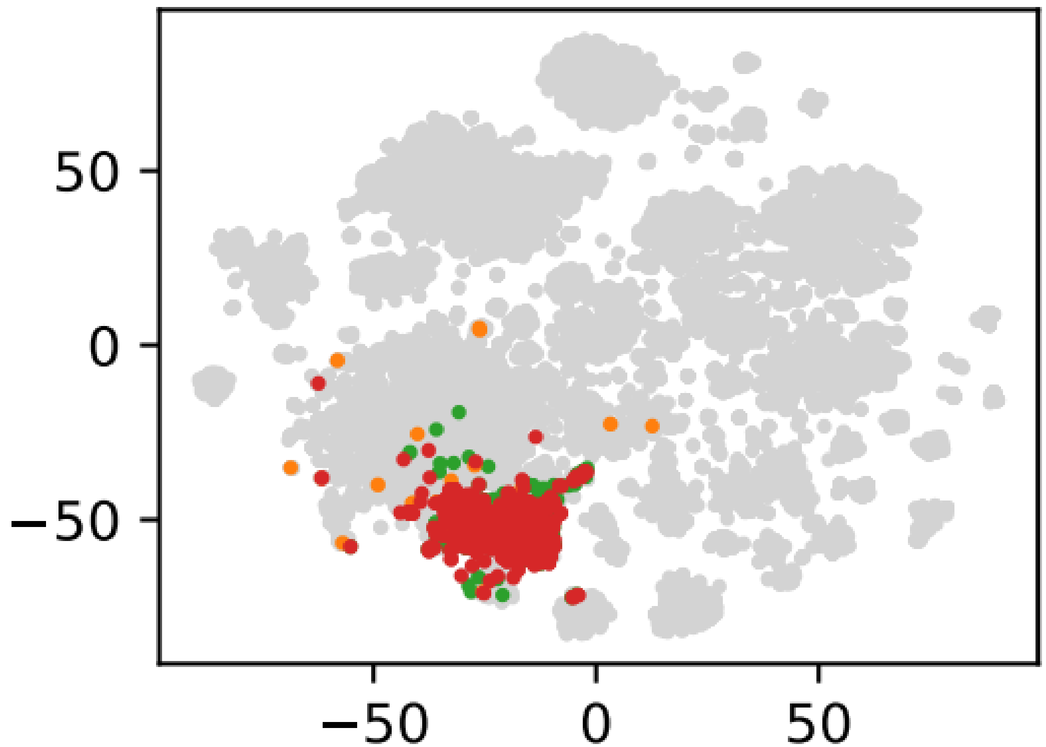
- TP
- FN
- FP
- TN

TPR: 100%
FPR: 0%

"List male instrumentalists who play <u>string instruments</u>"

String Instrument

Embedding Space



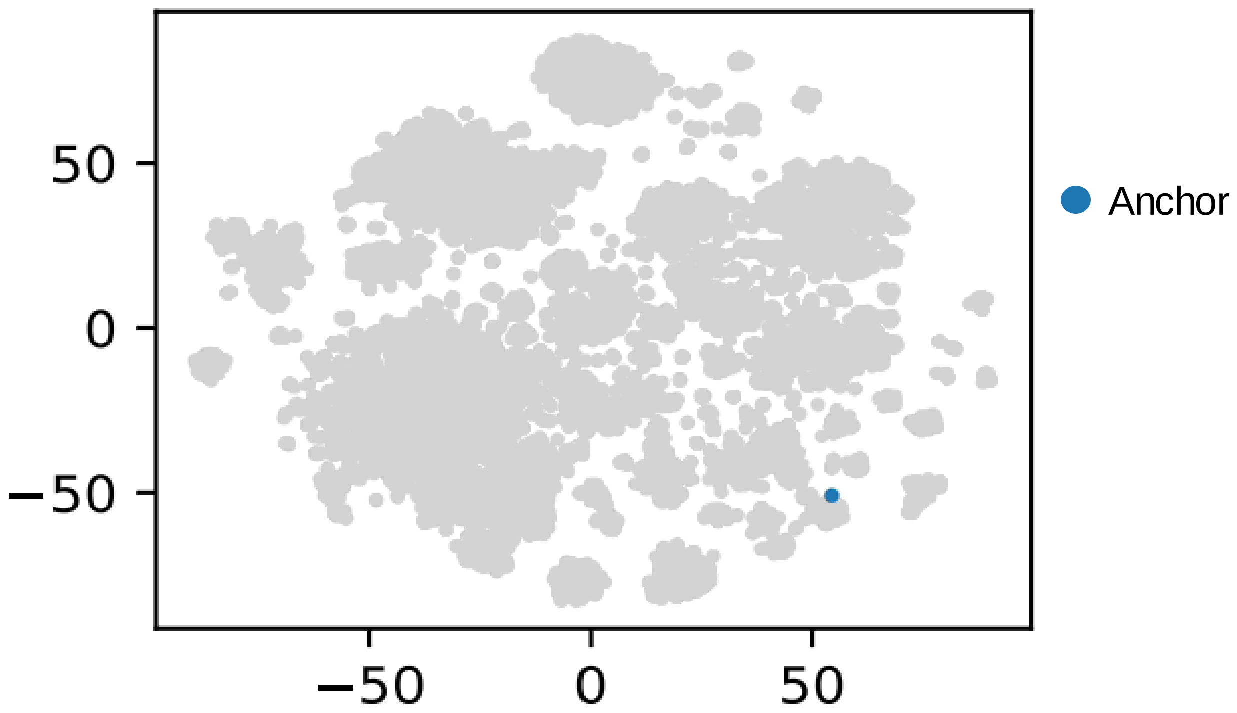
# of instrumentalists: 472

- TP
- FN
- FP
- TN

TPR: 98.4%
FPR: 0.01%

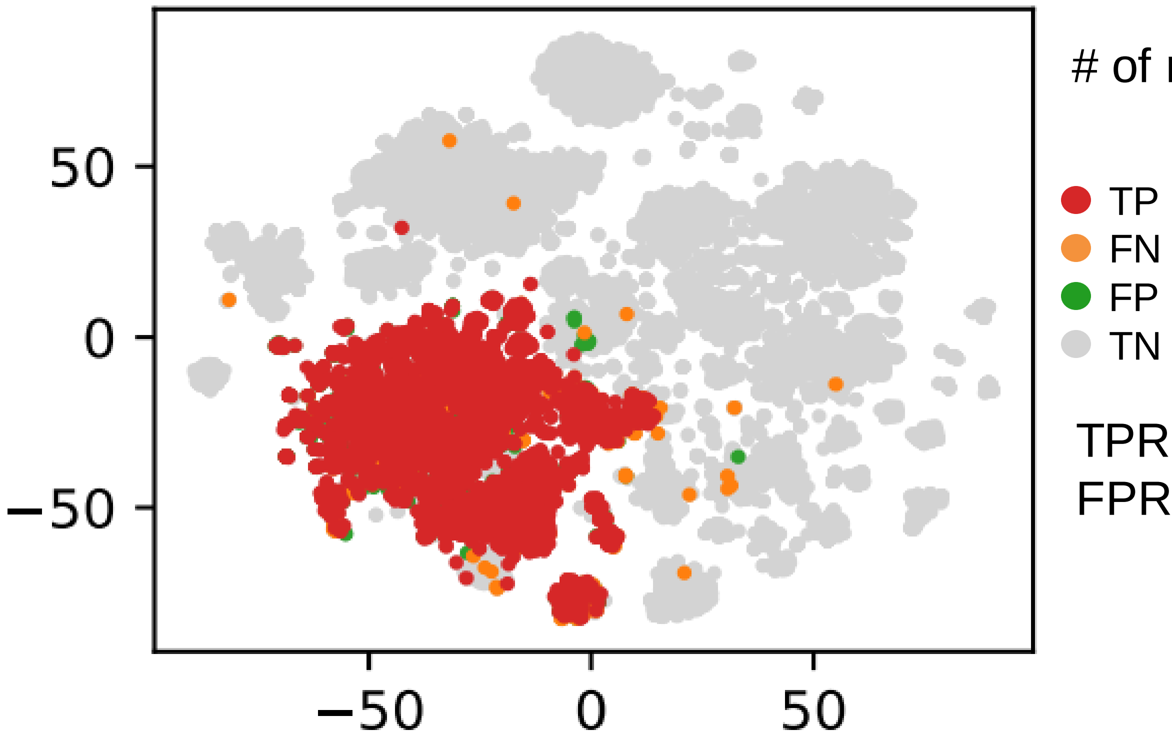
"List male <u>instrumentalists who play string instruments</u>"

Embedding Space



“List male instrumentalists who play string instruments”

Male

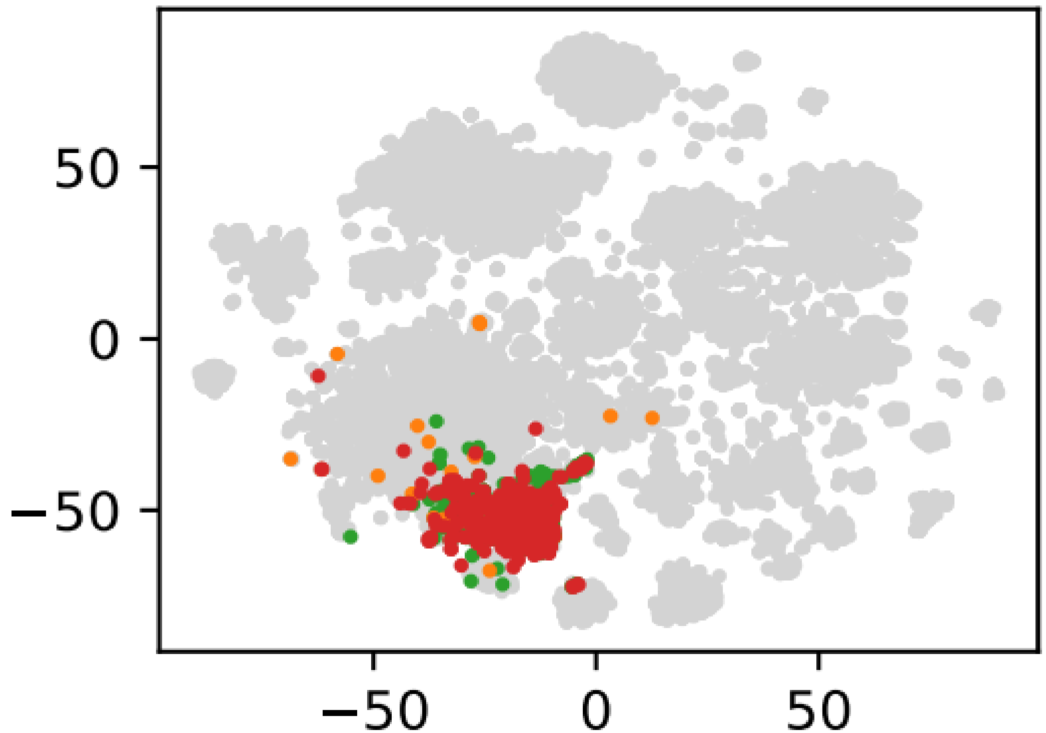


# of men: 3555

TPR: 97.9%
FPR: 0.01%

“List <u>male</u> instrumentalists who play string instruments”

Embedding Space

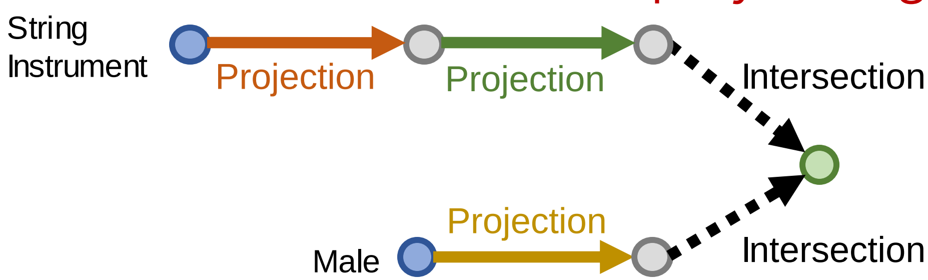


# of answers: 396

- TP
- FN
- FP
- TN

TPR: 99.4%
FPR: 0.01%

"List male instrumentalists who play string instruments"



Summary

- **We introduce answering predictive queries on large knowledge graphs.**
- **The key idea is to embed queries by navigating the embedding space!**
  - **We embed the query by composing learned operators**
  - **Embedding of the query is close to its answers in the embedding space**